

# Influence of magnetic boundaries scattering on order parameter and density of states of $^3\text{He}$ in confined geometry.

by

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### **Declaration of Authorship**

I, Evgeny Egorov, hereby declare that this thesis and the work presented in it is entirely my own. Where I have consulted the work of others, this is always clearly stated.

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## Abstract

This thesis is concentrated on investigating the effect of the boundary conditions on p-wave superconductivity/superfluidity. The first part of the thesis discusses a possibility of creating a Josephson effect as a result of the geometry of the sample. The second part continues work on a theoretical investigation of  $^3\text{He}$  in a confined geometry. To approach these problems theoretically a Ginzburg-Landau theory of second order transitions was used, while for the second part a quasiclassical approach was established. For the first problem gap profiles for various opening angles were obtained allowing to build a final plot with Josephson current magnitude dependence on the configuration of the gap on the two sides of Josephson junction. For the second problem, self-consistent order parameter profiles and local densities of states were obtained for various spin-mixing angles. A value of the parameter that nullifies the confinement effect on  $^3\text{He}$  was found, allowing for B-phase to be stable in a slab. Also presented a discussion of other possible outcomes of magnetic scattering at the boundaries on spectral densities of states, such as stabilization of the polar phase and the extension of the zero energy states area of existence across the Fermi surface up to the equator of the sphere( $p_z = 0$ ).

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# Chapter 1

## Introduction.

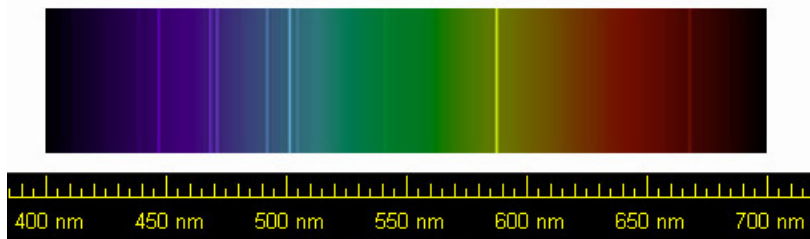
Quite often an explanation of the newest research requires a historical prospective of such. In case of a research in the field of a superconductivity, it is common to start with the discovery of the superconductivity and subsequent development of the theory describing it. Seeing that my research is centred around a certain unique material it would be only fair to start a bit earlier.

Among the many problems considered in physics there was, and might always be a problem of obtaining new states of matter. Physicists in the 19th century were especially interested in liquefying atmospheric gases. The first attempts were done by applying pressure to the pure gases and diverting heat produced in such process by any means possible. Particularly such process was used by Raoul Pictet in 1877 to liquefy oxygen, but he was outrun by Louis Paul Cailletet in this endeavour by a few days. While Cailletet's technique was not diverting any heat it allowed for actual observation of a process in which he demonstrated droplets of liquid condensing for a few seconds in a tube after pressure is released. On the other hand, Pictet in his experiment produced a considerable amount (about 22 cubic centimetres) of liquid and his experimental setup became a crucial foundation in further attempts of liquefying gases. As the experiments progressed, lighter and lighter gases were liquefied.

Soon enough physicists realized that with liquid gases they are not only discovering a liquid state of a known gas, but they also attain temperature regions that were unreachable to anyone on Earth before. So the new ultimate goal was to liquefy the lightest known gas to obtain the lowest temperature possible. This was achieved by Sir James Dewar in 1898. Initially, he

believed that in his experiments he also liquefied helium as it has higher atomic mass than hydrogen, but later on, it became clear that this was not the case and lower temperatures are yet to be achieved.

Here I want to take a small sidestep from low temperature physics discussion and briefly cover the discovery of helium. In the past, the conventional way to obtain an element was to run it through a sequence of chemical reactions extracting the element as a product of them. This approach would leave helium and other inert gases out of scope as they do not participate in any reactions under normal conditions. On the other hand, in the middle of the 19th century physicists started to measure radiation of various objects and established that the obtained spectrum is unique for each compound and varies with the body's temperature. In 1879 this phenomenon was formulated as a law by Joseph Stefan and later explained theoretically by Ludwig Boltzmann. Upon measuring the Sun's spectrum in 1868 independently by Jules Jansen and Norman Lockyer a bright yellow line was observed, and after ruling out all other possibilities, it was proposed that the line is produced by a new element which was called helium. Having been discovered in the solar corona helium was thought to be absent on Earth



**Figure 1.1:** Helium spectrum. A bright yellow line can be easily seen.

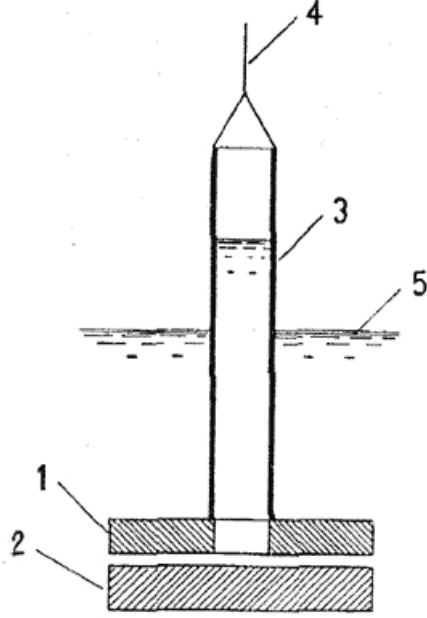
until it was isolated from cleveite by Sir William Ramsay in 1896. Since then, we know that helium in very small quantities exists in the Earth's atmosphere. Main helium production comes as a by-product of natural gas extracted from the earth where it can take up to 7% of the volume. Other natural sources of helium are minerals containing radioactive metals such as samarskite, cleveite, monazite.

The competition, to liquefy helium first, was won by Heike Kamerlingh Onnes in 1908 [2]. This success was a product of a long-time planning and the ability to create conditions needed for experimental work advancement. As an example of this in 1901, he initiated a glass blower workshop as a branch of his laboratory. This enabled the production of various experimental

equipment of a high quality and allowed to repeat Dewar achievement of liquefying hydrogen, but now the setup was able to produce a few litres of liquid hydrogen per day. The only obstacle was obtaining sufficient amounts of helium gas, which luckily, he was able to overcome by heating of monazite.

Upon conducting the experiment they could not see the liquid helium because a meniscus was almost absent, and the density of obtained liquid seemed to be lower than the expected value. The next logical step would be to obtain lower temperatures at which helium would solidify, but for reasons outside of classical theory that could not be done at low pressures. Despite failing attempts to solidify helium, Onnes got access to temperature regions never investigated before, enabling him to start testing various solid state theories at low temperatures. One of them was a temperature dependence of resistivity. It was believed by Onnes that resistivity at low temperatures should have linear dependence and be zero at zero temperature, however, his first measurements had shown it to become constant. Rightfully claimed by Onnes, the behaviour could be explained by the presence of impurities in the samples, so he decided to measure the resistivity of mercury as it could be made very clean. In 1911 he cooled down mercury under a temperature of 4.2K and found that the resistance of that metal falls drastically to a very small value that he was not able to distinguish from zero [3] in his experiment. Subsequent experiments unveiled other features of the phenomena later called by Onnes superconductivity.

It took almost 30 years for the experiments of Onnes to be revisited, and the significance of the phenomenon to be realized. In 1938 Pyotr Kapitsa published a note and later a paper [4] where he conducted an experiment measuring the viscosity of a liquid helium below 2.1K. Upon conducting the experiment he put an upper boundary for helium's viscosity to be  $10^{-9}$  C.G.S. units and proposed to call this phenomenon in analogy to superconductivity - superfluidity. These 30 years of difference was not a coincidence neither. At the time of Onnes works, quantum mechanics just started its development and an adequate atomic model was just on its way. Consequently, at the time it was nearly impossible to answer why helium liquefies at temperatures lower than hydrogen or why the meniscus almost completely disappears for the liquid, however, by 1938 quantum mechanics was already formulated mathematically and many predictions and advanced models crucial for an understanding of the problem were done. One of such models appeared in 1924-1925. Satyendra Nath Bose and Albert Einstein [5] formulated



**Figure 1.2:** Scheme of experiment used by Kapitsa to determine flow in Helium and its decay rate.

an idea of a quantum state of a matter when a gas of weakly interacting particles with integer spin at temperatures close to absolute zero behave as a whole. These particles, which were later called Bosons, occupy energy levels, according to Bose-Einstein statistics, which allow multiple particles to be in the same state. At low temperatures, a major fraction of these particles occupies the lowest energy state, which allows treating the gas as a macroscopic quantum system described by a single particle wave function. In 1938, Bose-Einstein condensation was proposed as a mechanism of superfluidity by Fritz London [6].

Approximately at the same time a new isotope of He was identified by Mark Oliphant [7] in 1934. For a long time, it was thought to be unstable until it was found in samples of natural helium. Unlike its most common isotope, the rarer isotope  $^3\text{He}$  is a fermion, making it a perfect candidate for a model system to understand superconductivity in metals. Having the advantages of being system of only fermions which is not obscured by interactions with a lattice, and also being remarkably pure, should have made it a priority system to investigate if it were not for one major setback. Natural abundance of  $^3\text{He}$  is 0.000137% of He. Consequently, obtaining sufficient amounts of  $^3\text{He}$  seemed impossible at that time.

At the beginning of 1950s physicists came very close to the understanding of the supercon-

ductivity. There are a few discoveries that are believed to play a crucial role in the development of the microscopic theory of superconductivity.

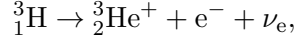
- Heat capacity in the superconducting state depends exponentially on temperature. This suggests an energy gap for particles dominating dynamics of the system at a superconducting temperature. For the reason that the divergence happens for the second derivative with respect to the temperature (heat capacity) of the corresponding energy functional one can deduce that the system experiences the second order phase transition in that point.
- Isotope effect was discovered in mercury in 1950 [8]. It turns out that the transition temperature depends on the mass of atoms comprising a lattice of the superconductor. This implies that the lattice also plays its role in this phase transition.

These facts point to a mechanism similar to Bose-Einstein condensation but miss a key feature. The superfluid theory is based on the fact that the particles composing the system are bosons, while clearly in metals holes and electrons are responsible for conduction. The fact that a lighter mass of lattice atoms corresponds to a higher critical temperature leads to the conclusion that lattice vibrations should be involved. At this point, it seems anyone could have come up with the microscopic theory of superconductivity, but most of the scientists working on that problem knew quantum physics too well.

In quantum physics, there is a textbook problem of a particle and its energy levels in a finite potential. Depending on the dimension of the problem one finds out that there is always an energy level for a bound state in one and two dimensions, however, it is not always the case in three. An assumption made by most was that a problem of two electrons interacting via virtual phonons is three-dimensional, and the potential created via this interaction wasn't strong enough to contain an energy level for a localized state. A breakthrough was made in 1956 by L. Cooper [9] where he considered a possibility of two electrons forming a pair if their momenta lie within close vicinity of a Fermi sphere. This assumption turned the considered model essentially two-dimensional and, as has been shown in the paper, allowed for a bound state to exist with the assumption that at some radius the interaction between two electrons is attractive. In 1957 a paper by J. Bardeen, L. Cooper, and J. R. Schrieffer formulated the microscopic theory [10] that is known as the BCS theory today. In the BCS theory, electrons

were assumed to form pairs with total zero spin and angular momentum respectively called "s-wave" pairing.

By the late 1950s, many countries were developing or already successfully developed their nuclear programs. As a result of a reaction at nuclear generating stations tritium could be produced. Helium-3, consequently, is a result of a tritium decay:



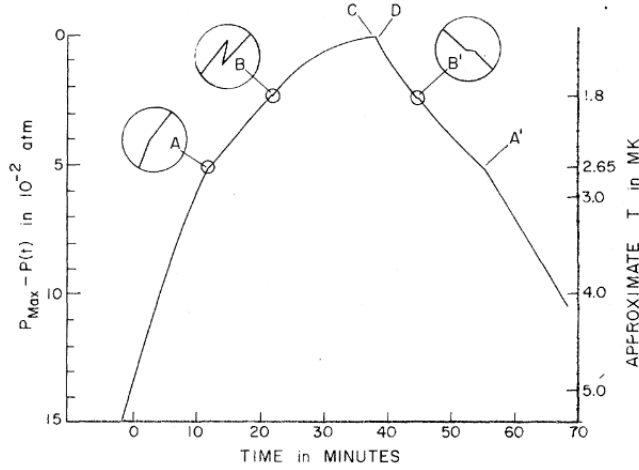
where an electron and an electron-neutrino are created as a by-product. Since then scientists have been able to obtain sufficient amounts of  ${}^3\text{He}$  both for study and cryogenics. This immediately posed a question if  ${}^3\text{He}$  superconducting and what properties it has.

Unlike many other examples in science this time theorists were the first to give an answer to a nature of superfluidity and Cooper pairing in  ${}^3\text{He}$ .

The main difference in  ${}^3\text{He}$  that was quickly realised is that a "Cooper pair" consists rather not of pairs of atoms, but rather of excitations above the Fermi sea. This results in an effective mass of the pairs to be considerably bigger than the mass of two  ${}^3\text{He}$  atoms because each atom "drags" a polarization cloud of surrounding atoms with itself. The second difference is that strong repulsion at a short distance in the quasiparticle effective potential results in a coupling with non-zero angular momentum. The corresponding pair wave-function vanishes at a zero relative distance, thus making the repulsive part of the potential ineffective. The Cooper pair wave function in conventional metals is spherically symmetric and called s-wave in analogy to an atom electron subshell's names. An s-wave Cooper pair due to having a zero angular momentum is not susceptible to the boundaries of a superconductor. On the contrary, a Cooper pair with a non-zero angular momentum can be destroyed during a scattering process which results in a modification of the superconductor's order parameter near boundaries. Anderson and Morell [11,12] in 1960 and 1961 respectively published a paper where they discussed the possibility of non-s-wave pairing states. Particularly, they focused on d-wave but also introduced "axial" p-wave state that was later called Anderson-Brinkman-Morel (ABM) state. This state has a feature that the energy gap  $\Delta$  has nodes (points where  $\Delta = 0$ ) on the Fermi surface with the orbital-angular momentum projection pointing along the direction of these nodes. The ABM state spin structure consists of two types of pairs with



$S_z = \pm 1$ . Clearly, a general p-wave state should consist of all three possible projections of momentum. Soon enough independently by Vdovin [13] and Balian and Werthamer [14] has been found an energetically favoured state with the equal mixing of all three spin components and uniform energy gap across the Fermi surface. By 1972 experimentalists had been able to reach the required temperature region and two phase transitions at 2.6 mK and 1.8 mK were observed by Osheroff D, Richardson R and Lee D [15]. These results inspired experimentalists



**Figure 1.3:** Observed pressure drop in solid-liquid  $^3\text{He}$  system. Feature A clearly suggests a second order transition which was affiliated with liquid by following experiments.

to investigate liquid  $^3\text{He}$  more extensively and so did theorists.

From theory perspective  $^3\text{He}$  is a perfect model system with a lot of intricate phenomena occurring in it such as a chiral current emerging on the system boundaries [16], or deep analogy to high energy physics [17]. For a deeper discussion on  $^3\text{He}$  properties and discovery history, I would reference the book by D. Vollhardt and P. Wolfe in [18]. This book is strongly recommended for the study to anyone somehow connected to the fields of superfluidity, superconductivity and phase transitions.

My research is inspired by one particular phenomenon. It seems that interest towards this topic started with a publication by M. Stone and R. Roy [19] where they discussed the possibility of Majorana-Weyl fermions in  $^3\text{He}$ -A phase. A little bit later came out a paper by A. Vorontsov and J. Sauls [1] where they showed that in constricted geometry  $^3\text{He}$  takes a new phase, which breaks the translational symmetry and consists from patches of B-phase that were alternating their  $\Delta_{Zz}$  component of order parameter separated by some kind of "domain

walls". Here the capital letters stand for a spin component of the order parameter and small letters stand for an orbital component. This, in turn, inspired a paper by K. Nagai, Y. Nagato, M. Yamamoto and S. Hugashitani [20] where they suggested that fermion zero-energy states exist and that a domain wall can be modelled just by the addition of specular boundaries in the system. Consequently, Volovik [21,22] considered a problem where a component of the order parameter changes sign when continuously varying along the trajectory. Which allows for the existence of a zero-energy state at the point where the previously mentioned component turns to zero. The wave-function describing that state would be self-conjugate meaning that this state would be an anti-particle of itself.

By now a Majorana fermion has been observed in a system with the quantum Hall effect [23]. There is an attempt to probe Majorana states with controlled impurities [24]. In my research, I want to consider a slightly different case. It has been shown that boundaries play a defining role in the existence of zero-energy modes in  $^3\text{He-B}$  systems. Apart from a stripe phase that occurs in a slab of finite width  $d$  when the width is approximately  $d = 10\xi_0$ , it is known [1,25] that the slab's thickness changes the stability of the  $^3\text{He}$  phases, with  $^3\text{He-A}$  existing for the width of a slab  $d < 10\xi_0$  and  $^3\text{He-B}$  phase in the opposite case.

In light of the above publications, the order parameter behaviour near a plane boundary is known. It would be interesting to investigate phenomena occurring due to a deviation of the boundary linearity. In particular, due to the interplay between the behaviour of the order parameter at the intersection of the two plane boundaries. Consequently, I want to consider the possibility of using the behaviour of p-wave superconductors near the boundaries as a way to alter the order parameter structure by managing the geometry of the considered system. As a way of demonstrating that hypothetical boundaries influence I suggest considering a Josephson junction where order parameter would be altered differently by the boundaries giving a rise to the Josephson effect.

A second direction to expand our knowledge of the p-wave system behaviour near the boundaries would be to consider a plane boundary condition, but with some special properties. For example, one can consider a boundary that not only reflects the momentum of quasiparticles but also adds additional phase to the spin part of the quasiparticles wave-function. This boundary conditions later are referred to as the magnetically active boundary conditions and usually are encountered in problems describing a Josephson effect for junctions

with magnetically active weak-link [26,27]. Introduction of that boundary conditions for  $^3\text{He}$  in a slab gave rise to a few phenomena that haven't been described in a literature before.

## Chapter 2

# Quasiclassical approach.

When one wants to give a full description of a superconducting state, there are two details that are essential to grasp. First, is to be able to fully describe the behaviour of conducting electrons in a normal state and, second, is being able to explain and account for coupling mechanism in the system of interest. In other words, the quasiclassical theory of superconductivity is a hybrid of two potent theories: Landau theory of Fermi Liquid and BCS theory. This construct is able to provide a description of considered superconductor or  $^3\text{He}$  superfluid at all temperature ranges and excitation energies within a field of interest. It is valid in both clean and dirty cases and covers even metal with strong electron-phonon and electron-electron interactions.

Fermi liquid theory was built by Landau in a series of papers [28, 29]. There he argued that any weak excitation of a system of strongly interacting electrons can be considered as a combination of elementary excitations which he called *quasiparticles*. These quasiparticles exist only inside considered system representing collective excitations in the system and determined by their energies  $\epsilon$  and momenta  $\mathbf{p}$ .

The BCS theory of superconductivity was formulated in the paper by Bardeen, Cooper and Schrieffer [10]. In that paper, they presented the microscopical mechanism that could explain the emergence of superconducting condensate in metals which in turn allowed to account for superconducting properties of a system in a similar way to superfluidity of  $^4\text{He}$ . Within next ten years, Eilenberger [30] and Larkin and Ovchinnikov [31] realised and shown that standard equilibrium theory of superconductivity can be formulated in terms of quasiclassical transport equations. A bit later this result was generalized to non-equilibrium conditions by Eliashberg

[32]. This theory is a generalisation of the Landau Fermi liquid theory to superconducting states. It combines Landau's semi-classical transport equations for quasiparticles with pairing and particle-hole coherence that are essential to BCS theory. Later in the chapter, this theory will be referred as *quasiclassical theory*.

## 2.1 Basics of the Fermi liquid theory.

As it would become clear later in this chapter the theory behind my research is concentrated on solving many-body problems in quantum mechanics. One of the first successful solutions to the problem of strongly interacting fermions was Fermi-liquid theory introduced by Landau [28]. This theory allows to obtain various thermodynamic properties of the system starting with the entropy. It also allowed to predict zero sound and spin-waves in the Fermi liquid system. Although system applicability criteria seem to be quite restricting  $T \ll T_F$  it turns out that for most metals this condition is fulfilled up to the melting temperatures. However, for the  $^3\text{He}$  superfluid the theory is inapplicable directly due to the emergence of a Cooper pairs in the system. For that reason, I will not go into details about predictive powers of that theory, but discuss the core concept in it that is wildly used in other theories describing superconducting/superfluid state of the system. The Fermi liquid theory starts with a postulate that every weak in comparison with  $E_F$  state of the system can be described as a multitude of elementary excitations of the system, that have an energy  $\xi$  and momentum  $\mathbf{k}$  and are called *quasiparticles*. In order to describe the system of the fermion quasiparticles a distribution function is introduced  $n_{\alpha\beta}(k)$  which obeys the normalisation condition:

$$\sum_{\alpha} \int n_{\alpha\alpha}(\mathbf{k}) \frac{d^3\mathbf{k}}{(2\pi\hbar)^3} = \frac{N}{V}$$

where  $N$  is total number of the quasiparticles in the system with the volume  $V$ . Similarly the quasiparticle energy can be defined as:

$$\frac{\delta E}{V} = \sum_{\alpha} \int \xi_{\alpha\beta}(\mathbf{k}) \delta n_{\alpha\beta}(\mathbf{k}) \frac{d^3\mathbf{k}}{(2\pi\hbar)^3}. \quad (2.1)$$

In the vicinity of the fermi energy the quasiparticle energy can be parametrised in the following way:

$$\xi_{\alpha\alpha}(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m^*} \approx \frac{\hbar^2 \mathbf{k}_F^2}{2m^*} + \hbar \mathbf{v}_F (\mathbf{k} - \mathbf{k}_F), \quad \mathbf{v}_F = \frac{1}{\hbar} \frac{\partial \xi(\mathbf{k})}{\partial \mathbf{k}},$$

the first term in the expression is the chemical potential  $\mu$ . Due to the fact that energy levels of the quasiparticle states has one-to-one correspondence with the states of the Fermi gas the entropy of the quasiparticle system is given by the same expression as the entropy of the Fermi gas:

$$\frac{S}{V} = -k_B \sum_{\alpha} \int n_{\alpha\alpha}(\mathbf{k}) \log(n_{\alpha\alpha}(\mathbf{k})) + (1 - n_{\alpha\alpha}(\mathbf{k})) \log((1 - n_{\alpha\alpha}(\mathbf{k}))) \frac{d^3 \mathbf{k}}{(2\pi\hbar)^3},$$

varying entropy with the boundary conditions that stand for the constant number of quasiparticles and total energy:

$$\frac{\delta N}{V} = \sum_{\alpha} \int \delta n_{\alpha\alpha}(\mathbf{k}) \frac{d^3 \mathbf{k}}{(2\pi\hbar)^3} = 0 \quad \frac{\delta E}{V} = \sum_{\alpha} \int \xi_{\alpha\beta}(\mathbf{k}) \delta n_{\alpha\beta}(\mathbf{k}) \frac{d^3 \mathbf{k}}{(2\pi\hbar)^3} = 0$$

we obtain:

$$n_{\alpha\beta}(\mathbf{k}) = \left[ e^{\frac{\xi_{\alpha\beta}(\mathbf{k}) - \mu}{k_B T}} + 1 \right]^{-1}.$$

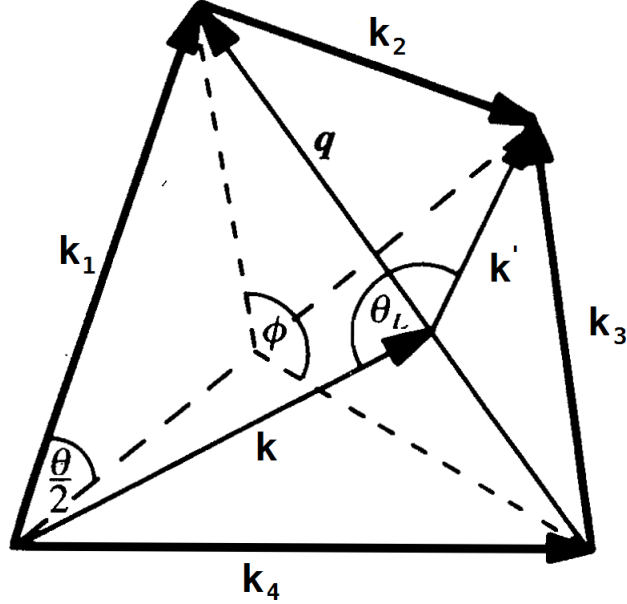
Strictly speaking it is not yet a Fermi distribution but an integral equation on the distribution function  $n_{\alpha\beta}(\mathbf{k})$  as the quasiparticle energy  $\xi_{\alpha\beta}(\mathbf{k})$  itself depends on the distribution function by definition 2.1.

Because quasiparticle states are not energy eigenstates before describing the system in quasiparticle terms we should find conditions when that description is applicable. Putting it simply we should derive an expression for the quasiparticles lifetime  $\tau$  and state that this time is sufficiently long to govern dynamics we try to describe. In order to do that we should consider quasiparticle interaction. At low temperatures  $T \ll T_F$  binary collisions will dominate and the lifetime of a quasiparticle with momentum  $\mathbf{k}$  and spin  $\alpha$  would obey the Golden Rule expression:

$$\frac{1}{\tau_{\mathbf{k}\alpha}} = \frac{2\pi}{\hbar} \sum_{234} |a(1, 2; 3, 4)|^2 n_2(1-n_3)(1-n_4) \delta_{\mathbf{k}1+\mathbf{k}2, \mathbf{k}3+\mathbf{k}4} \delta_{\alpha_1+\alpha_2, \alpha_3+\alpha_4} \delta(\xi_1+\xi_2-\xi_3-\xi_4). \quad (2.2)$$

Here delta functions stand for conservation of momentum, spin and energy during the scat-

tering process. The Fermi factors represent probability of state 2 being occupied and states 3 and 4 being empty. The transition probability is given by the square of the quasiparticle scattering amplitude  $a(1, 2; 3, 4)$  for the binary scattering process  $(1, 2) \rightarrow (3, 4)$ . Spin-rotation invariance implies that there are only two independent scattering amplitudes for reason that there are only two types of states describing pair of interacting fermions: singlet and triplet. Taking into account momentum preservation and rotation invariance in momentum space the quasiparticle scattering amplitude may be dependent only on two angular variables. Customarily these angles are chosen as  $\theta$  angle between the momenta of incoming particles i.e.  $\cos(\theta) = (\mathbf{k}_1, \mathbf{k}_2)$  and choice of angle  $\phi$  as angle between planes spanned by pairs of vectors  $\{\mathbf{k}_1, \mathbf{k}_2\}$  and  $\{\mathbf{k}_3, \mathbf{k}_4\}$  i.e  $\cos(\phi) = ([\mathbf{k}_1 \times \mathbf{k}_2], [\mathbf{k}_3 \times \mathbf{k}_4]) / ||[\mathbf{k}_1 \times \mathbf{k}_2]|| * ||[\mathbf{k}_3 \times \mathbf{k}_4]||$  as shown on the figure:



**Figure 2.1:** Graphical representation of the quasiparticle scattering amplitude in terms of the incoming and outgoing quasiparticle momentum vectors  $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4$ .

By introducing dimensionless scattering amplitudes  $A^{s,t}(\theta, \phi)$  for the singlet and triplet states respectively we can write:

$$a(1, 2; 3, 4) = \frac{1}{4N_F} \left[ (3A^t + A^s) \delta_{\alpha_1, \alpha_2} \delta_{\alpha_3, \alpha_4} + (A^t - A^s) \sum_{\nu} (\sigma_{\nu})_{\alpha_1 \alpha_3} \sum_{\nu} (\sigma_{\nu})_{\alpha_2 \alpha_4} \right], \quad (2.3)$$

where  $N_F$  is the density of states at the Fermi level defined as:

$$N_F = \sum_{\alpha} \int \delta(\xi_{\mathbf{k},\alpha} - \mu) \frac{d^3\mathbf{k}}{(2\pi\hbar)^3} = \frac{m^* k_F}{\pi^2 \hbar^2} \quad (2.4)$$

Transforming the sums over momenta in 2.2 into integrals over energy and angular variables and performing the integration we arrive to the expression:

$$\frac{1}{\tau_{\mathbf{k}\alpha}} = \left[ 1 + \left( \frac{\xi_{\mathbf{k}\alpha} - \mu}{\pi k_B T} \right)^2 \right] \frac{1}{\tau_N^0}, \quad (2.5)$$

where the  $\tau_N^0$  stands for the quasiparticle lifetime at the Fermi surface given by:

$$\tau_N^0 = \frac{64\hbar}{\pi^3} \frac{E_F}{k_B^2 T^2} \int_0^1 d(\cos(\frac{\theta}{2})) \int_0^{2\pi} \frac{d\phi}{2\pi} (|A^s|^2 + 3|A^t|^2). \quad (2.6)$$

As it can be observed from the formula the quasiparticle relaxation rate is proportional to the sum  $k_B T^2 + (\xi_{\mathbf{k}\alpha} - \mu)^2$ . This means that quasiparticles are sufficiently long lived excitations if the system considered at low temperatures and the energy of the excited system is not far away from the ground state energy. To conclude I would like to list the points that will help us build the microscopical theory of the superconductivity in the next section.

- The system of strongly interacting fermionic particles at sufficiently low temperatures  $T \ll T_F$  can be described by excitations of that system from the ground state called *quasiparticles*.
- These quasiparticles are sufficiently long living if their energy is close to the chemical potential  $|\xi_{\alpha\beta}(\mathbf{k}) - \mu| \rightarrow 0$
- In case of non-interacting quasiparticles, their distribution function is identical to such of the Fermi gas. This would happen if the described system Hamiltonian is diagonal in terms of quasiparticle creation and annihilation operators.



## 2.2 The BCS theory.

### 2.2.1 The Cooper problem.

Investigation of the properties of superconductors prior to BCS theory has revealed a couple of crucial facts about those systems. First, is the behaviour of the heat capacity far away from the transition point that obeyed the formula:

$$C_{sc} = c_1 T^3 + c_2 e^{\frac{E_{gap}}{k_B T}}.$$

The first term of that sum clearly accounts for phononic heat capacity while the second one closely resembles the heat capacity of the semiconductors. The second term is a telltale sign of a gap in the electronic spectrum of superconductors. The second fact is isotopic effect measured in mercury [8] which tells that lattice atom vibrations are important for the superconductivity in metals. This fact discards an idea of purely electronic superconductivity. The idea was based on a belief that in a superconducting state electrons would not interact with the lattice atoms explaining the zero resistivity. These two facts seemed to point out the similarity between superconductivity and superfluidity mechanism suggested by Landau [33] in 1941 for  $^4\text{He}$ . For a complete analogy, one would require for electrons to couple into the bosonic quasiparticles and interaction via phonons seems to be the mechanism if not for one detail. One can estimate an energy of attraction between the electrons as  $E_{int} \approx k_B T_c$  and the kinetic energy of electrons as  $E_{kin} \approx E_F$ . In the conventional superconductors the ratio  $E_{int}/E_{kin} \approx 10^{-3}$  meaning that the interaction is not strong enough to bound free electrons into pairs. This obstruction was resolved by L. Cooper [9]. Cooper considered an interacting pair of quasiparticles added to the system of  $N$  identical non-interacting fermions. We can consider a general case when the wave function of that system is given by the antisymmetrized product of an interacting pair wave-function  $\Phi(\mathbf{r}_1, \mathbf{r}_2, \alpha, \beta)$  and an  $N$ -particle Slater determinant describing the Fermi sea. The pair wave-function is a product of a centre of mass plane wave, relative motion wave-function  $\psi(\mathbf{r}_1 - \mathbf{r}_2)$  and a spin wave-function  $\mathcal{X}(\alpha, \beta)$ :

$$\Phi(\mathbf{r}_1, \mathbf{r}_2, \alpha, \beta) = e^{\frac{i\mathbf{P} \cdot (\mathbf{r}_1 + \mathbf{r}_2)}{2}} \psi(\mathbf{r}_1 - \mathbf{r}_2) \mathcal{X}(\alpha, \beta)$$

The most important effect from the Fermi sea is to occupy states all states below  $E_F$ . That can be taken into account by switching to the momentum representation. The Schrödinger equation for a pair wave-function in the momentum representation will read:

$$(\xi_{\mathbf{k}+\mathbf{P}/2} + \xi_{\mathbf{k}-\mathbf{P}/2} - E) \psi_{\mathbf{k}} = -\frac{1}{(2\pi)^{3/2}} \int_{\mathbf{k}' > \mathbf{k}_F} d^3\mathbf{k}' V_{\mathbf{k}-\mathbf{k}'} \psi_{\mathbf{k}'}. \quad (2.7)$$

The quasiparticle energy is measured from the Fermi level and defined here as:

$$\xi_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m} - \mu,$$

where  $\mu$  stands for the chemical potential. It is clear from 2.7 that the lowest energy is obtained for the two particles and oppositely directed momenta. The equation can be separated into angular-momentum components by expanding the interaction potential in terms of Legendre polynomials  $P_l(\mathbf{k} \cdot \mathbf{k}')$  and spherical harmonics  $Y_{lm}(\mathbf{k})$  and will read:

$$V_{\mathbf{k}-\mathbf{k}'} = \sum_{l=0}^{\infty} (2l+1) V_l(k, k') P_l(\mathbf{k} \cdot \mathbf{k}'),$$

$$\psi_{\mathbf{k}'} = \sum_{lm} \psi_l(k) Y_{lm}(\mathbf{k}).$$

Assuming that  $V_l$  is a constant within a thin shell near the Fermi energy allows to obtain the analytical solution to 2.7 by solving the equation:

$$(2\xi_{\mathbf{k}} - E) \psi_l(k) = -V_l N(0) \int_0^{e_c} \psi_l(k') d\xi_{\mathbf{k}'}.$$

here the density of states  $N(0)$  is taken out of the integral as considered to be slowly varying on the scale of the cut-off energy  $e_c$ . The obtained equation is identical to a problem of two scattering particles in two dimensions. By observation one can see that for the attractive interaction  $V < 0$  the energy eigenvalue  $E$  is negative which corresponds to a bound state for an arbitrarily weak interaction. The pairing happens for the biggest coefficient  $V_l$  thus defining the relative angular momentum of the Cooper pair.

### 2.2.2 The BCS theory in the Bogolubov approach.

Realisation of the fact that formation of the Cooper pairs is energetically profitable allows to consider the following Hamiltonian of the system of interacting quasiparticles:

$$\begin{aligned}
 H - \mu N &= \sum_{\mathbf{k}, \alpha} \xi_{\mathbf{k}, \alpha} a_{\mathbf{k}, \alpha}^\dagger a_{\mathbf{k}, \alpha} + \\
 &+ \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \sum_{\alpha, \beta, \alpha', \beta'} \langle -\mathbf{k}\alpha, \mathbf{k} + \mathbf{q}\beta | V | \mathbf{k}'\alpha', -\mathbf{k}' + \mathbf{q}\beta' \rangle a_{\mathbf{k}', \alpha'}^\dagger a_{-\mathbf{k}' + \mathbf{q}, \beta'}^\dagger a_{-\mathbf{k}, \alpha} a_{\mathbf{k} + \mathbf{q}, \beta}, \\
 \xi_{\mathbf{k}, \alpha} &= \xi_{\mathbf{k}} - \alpha \mu_0 H
 \end{aligned}$$

Because only the pairs of particles with equal and opposite momenta are correlated and the correlation phenomena is of dominant importance in that problem we will simplify the interaction term by introducing average of the  $a_{-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger$  operators. This step turns BCS into a mean-field theory as an interaction of a Cooper pair with other pairs there substituted by the mean field  $\Delta_{\mathbf{k}, \alpha, \beta}$ . Then, the problem Hamiltonian will take form:

$$H - \mu N = \sum_{\mathbf{k}, \alpha} \xi_{\mathbf{k}, \alpha} a_{\mathbf{k}, \alpha}^\dagger a_{\mathbf{k}, \alpha} + \frac{1}{2} \sum_{\mathbf{k}, \alpha, \beta} \Delta_{\mathbf{k}\alpha\beta}^* a_{-\mathbf{k}\beta} a_{\mathbf{k}\alpha} + a_{\mathbf{k}\alpha}^\dagger a_{-\mathbf{k}\beta}^\dagger \Delta_{\mathbf{k}\beta\alpha} - \frac{1}{2} \sum_{\mathbf{k}, \alpha, \beta} \Delta_{\mathbf{k}\alpha\beta}^* P_{\mathbf{k}\alpha\beta}, \quad (2.8)$$

where two new quantities has been defined:

$$\begin{aligned}
 \Delta_{\mathbf{k}\alpha\beta} &= -\Delta_{-\mathbf{k}\beta\alpha} = \sum_{\mathbf{k}', \alpha', \beta'} \langle -\mathbf{k}\alpha, \mathbf{k}\beta | V | \mathbf{k}'\alpha', -\mathbf{k}'\beta' \rangle P_{\mathbf{k}', \alpha', \beta'} \\
 \langle a_{-\mathbf{k}\beta} a_{\mathbf{k}\alpha} \rangle &= \delta_{\mathbf{k}, \mathbf{k}'} P_{\mathbf{k}, \alpha, \beta}
 \end{aligned} \quad (2.9)$$

and  $\langle \cdot \rangle$  stands for average over the pair wave-function. Given form of the Hamiltonian 2.8 contains non-diagonal terms  $a_{-\mathbf{k}} a_{\mathbf{k}}$  and  $a_{-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger$  which results in our inability to solve corresponding Schrödinger equations. In order to avoid that issue a digonalization procedure was implemented by Bogolubov [34]. The main idea of that procedure is to find a linear combination of creation and annihilation operators that will turn the BCS theory Hamiltonian

diagonal. The new operators will be related to the old ones by the formulas:

$$b_{\mathbf{k}\alpha} = \sum_{\beta} u_{\mathbf{k},\alpha,\beta} a_{\mathbf{k}\beta} - v_{\mathbf{k},\alpha,\beta} a_{-\mathbf{k}\beta}^{\dagger} \quad b_{\mathbf{k}\alpha}^{\dagger} = \sum_{\beta} u_{\mathbf{k},\alpha,\beta}^* a_{\mathbf{k}\beta}^{\dagger} - v_{\mathbf{k},\alpha,\beta}^* a_{-\mathbf{k}\beta}. \quad (2.10)$$

For this substitution to work the new operators should satisfy the anti-commutation relations:

$$\begin{aligned} \{b_{\mathbf{k}\alpha}, b_{\mathbf{k}'\beta}^{\dagger}\} &= \delta_{\alpha,\beta} \delta_{\mathbf{k},\mathbf{k}'}, \\ \{b_{\mathbf{k}\alpha}, b_{\mathbf{k}'\beta}\} &= \{b_{\mathbf{k}\alpha}^{\dagger}, b_{\mathbf{k}'\beta}^{\dagger}\} = 0. \end{aligned}$$

These relations in turn force a certain conditions on the coefficients  $u_{\mathbf{k},\alpha,\beta}$  and  $v_{\mathbf{k},\alpha,\beta}$ , which are formulated in the matrix form:

$$\begin{aligned} \hat{u}_{\mathbf{k}} \hat{u}_{\mathbf{k}}^{\dagger} + \hat{v}_{\mathbf{k}} \hat{v}_{\mathbf{k}}^{\dagger} &= 1 \\ \hat{u}_{\mathbf{k}} \hat{v}_{\mathbf{k}} - \hat{v}_{\mathbf{k}} \hat{u}_{\mathbf{k}} &= 1 \end{aligned} \quad (2.11)$$

Using relations 2.11 and making the substitution 2.10 into the Hamiltonian 2.8 with the condition that the resulting form of the Hamiltonian should be diagonal in terms of the new creation and annihilation operators one would obtain following condition on the coefficients:

$$2\xi_{\mathbf{k}} \hat{u}_{\mathbf{k}} \hat{v}_{\mathbf{k}} - \hat{v}_{\mathbf{k}} \hat{\Delta}_{\mathbf{k}}^{\dagger} \hat{v}_{\mathbf{k}} + \hat{u}_{\mathbf{k}} \hat{\Delta}_{\mathbf{k}} \hat{u}_{\mathbf{k}} = 0, \quad (2.12)$$

where  $\hat{\Delta}_{\mathbf{k}}$  is  $2 \times 2$  matrix constructed out of previously introduced quantity  $\Delta_{\mathbf{k}\beta\alpha}$ . This equation 2.12 on the amplitudes  $\hat{u}_{\mathbf{k}}$  and  $\hat{v}_{\mathbf{k}}$  with the help of 2.11 can be transformed to a set of the Ricatti equations. The algorithm to solve that type of equations will be discussed later, while here we will just use the answer:

$$\begin{aligned} u_{\mathbf{k},\alpha,\beta} &= \delta_{\alpha\beta} \frac{\xi_{\mathbf{k}\alpha} + \Omega_{\mathbf{k}\alpha}}{\sqrt{2\Omega_{\mathbf{k}\alpha} (\xi_{\mathbf{k}\alpha} + \Omega_{\mathbf{k}\alpha})}}, \quad v_{\mathbf{k},\alpha,\beta} = \frac{-\Delta_{\mathbf{k},\alpha,\beta}}{\sqrt{2\Omega_{\mathbf{k}\alpha} (\xi_{\mathbf{k}\alpha} + \Omega_{\mathbf{k}\alpha})}} \\ \Omega_{\mathbf{k}\alpha} &= \sqrt{\xi_{\mathbf{k}\alpha}^2 + \left( \hat{\Delta}_{\mathbf{k}} \hat{\Delta}_{\mathbf{k}}^{\dagger} \right)_{\alpha\alpha}} \end{aligned} \quad (2.13)$$

Here one can check by direct calculation that  $\hat{\Delta}_{\mathbf{k}}\hat{\Delta}_{\mathbf{k}}^\dagger$  will always be a diagonal matrix. Substituting the obtained solution 2.13 into the Hamiltonian we obtain:

$$H - \mu N = \sum_{\mathbf{k}\alpha} \frac{1}{2} \left( \hat{\Delta}_{\mathbf{k}} \hat{\Delta}_{\mathbf{k}}^\dagger \right)_{\alpha\alpha} \left( \frac{1}{2\Omega_{\mathbf{k}\alpha}} - \frac{1}{\xi_{\mathbf{k}\alpha} + \Omega_{\mathbf{k}\alpha}} \right) + \Omega_{\mathbf{k}\alpha} b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha} \quad (2.14)$$

From the Hamiltonian we can obtain the single-particle excitation energy:

$$E(\mathbf{k}, \alpha) = \Omega_{\mathbf{k}\alpha} = \sqrt{\left( \frac{\hbar^2 \mathbf{k}^2}{2m^*} - \mu \right)^2 + \sum_{\beta} \Delta_{\mathbf{k}\alpha\beta} \Delta_{\mathbf{k}\alpha\beta}^*} \quad (2.15)$$

From the formula one can see that the energy spectrum doesn't go to zero but remains finite. The minimum of that energy is found when  $k = k_F$  and equals  $|\Delta|$ , which explains why the superconducting order parameter is known as the "gap parameter".

### 2.2.3 The Gap equation.

The Bogolubov quasiparticles are non-interacting fermions. At the finite temperature these states are occupied according to the Fermi statistics, which means:

$$\langle b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}'\beta} \rangle_T = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\alpha\beta} f_{\mathbf{k}\alpha} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\alpha\beta} \frac{1}{e^{\frac{E(\mathbf{k},\alpha)}{k_B T}} + 1},$$

where  $\langle \cdot \rangle_T$  stands for the thermal average of the operator inside the brackets. Using the Bogolubov transformation 2.10 we can calculate average of the electronic operators via known average of the Bogolubov quasiparticles.

$$\begin{aligned} \langle a_{\mathbf{k}\alpha}^\dagger a_{\mathbf{k}\alpha} \rangle_T &= \frac{1}{2} \left( 1 + \frac{\xi_{\mathbf{k}\alpha}}{\Omega_{\mathbf{k}\alpha}} \right) f_{\mathbf{k}\alpha} + \frac{1}{2} \left( 1 - \frac{\xi_{\mathbf{k}\alpha}}{\Omega_{\mathbf{k}\alpha}} \right) (1 - f_{\mathbf{k}\alpha}) \\ P_{\mathbf{k}\alpha\beta} &= \langle a_{-\mathbf{k}\beta} a_{\mathbf{k}\alpha} \rangle_T = -\frac{\Delta_{\mathbf{k}\alpha\beta}}{2\Omega_{\mathbf{k}\alpha}} (1 - 2f_{\mathbf{k}\alpha}) \end{aligned} \quad (2.16)$$

Substituting obtained formula 2.16 into the definition for the  $\Delta_{\mathbf{k}\alpha\beta}$  we obtain:

$$\Delta_{\mathbf{k}\alpha\beta} = - \sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} \frac{\Delta_{\mathbf{k}'\alpha\beta}}{2\Omega_{\mathbf{k}'\alpha}} \tanh \left( \frac{\Omega_{\mathbf{k}'\alpha}}{2k_B T} \right) \quad (2.17)$$

Here I substituted the matrix element of the interaction potential from 2.9 for the interaction function  $V_{\mathbf{k}-\mathbf{k}'}$  the following way:

$$\langle -\mathbf{k}\alpha, \mathbf{k}\beta | V | \mathbf{k}'\alpha', -\mathbf{k}'\beta' \rangle = \delta_{\alpha\alpha'} \delta_{\beta\beta'} V_{\mathbf{k}-\mathbf{k}'}$$

This substitution is viable as the variation of the interaction potential  $V_{\mathbf{k}-\mathbf{k}'}$  occurs on a scale of the Fermi momentum which is large compared to the Cooper pair momenta of the order  $\Delta/p_F$ . This happens because  $T_c/T_F$  is relatively small in most of the superconductors. That fact also means that the order parameter momentum dependence is in most cases dictated by the single most attractive channel in decomposition of the interaction function  $V_{\mathbf{k}-\mathbf{k}'}$  by spherical harmonics. This allows to assume that the function is approximated by the following formula:

$$V_{\mathbf{k}-\mathbf{k}'} = \begin{cases} (2L+1)V_L P_L(\mathbf{k} \cdot \mathbf{k}'), & |e_{\mathbf{k}}|, |e_{\mathbf{k}'}| < e_c \\ 0, & |e_{\mathbf{k}}|, |e_{\mathbf{k}'}| \geq e_c \end{cases}$$

In the assumption of the zero external magnetic field we can assume  $\xi_{\mathbf{k}\alpha} = \xi_{\mathbf{k}}$  and then the gap equation would read:

$$\Delta_{\mathbf{k}\alpha\beta} = -(2L+1)V_L N(0) \left\langle P_L(\mathbf{k} \cdot \mathbf{k}') \Delta_{\mathbf{k}'\alpha\beta} \int_0^{e_c} d\xi_{\mathbf{k}'} \frac{\tanh\left(\frac{\Omega_{\mathbf{k}'\alpha}}{2k_B T}\right)}{\Omega_{\mathbf{k}'\alpha}} \right\rangle_{\frac{\mathbf{k}'}{|\mathbf{k}'|}}, \quad (2.18)$$

where summation over all momenta  $\mathbf{k}$  is separated into angular average integral  $\langle \cdot \rangle_{\frac{\mathbf{k}'}{|\mathbf{k}'|}}$  and integral over the momenta values  $\sum_{|\mathbf{k}|} \approx N(0) \int_0^{e_c} d\xi_{\mathbf{k}}$ . For the case of s-wave order parameter when  $\Delta_{\mathbf{k}\alpha\beta}$  is independent from the quasiparticle momenta the expression 2.18 simplifies to a well-known formula:

$$1 = -V_L N(0) \left\langle \int_0^{e_c} d\xi_{\mathbf{k}'} \frac{\tanh\left(\frac{\Omega_{\mathbf{k}'\alpha}}{2k_B T}\right)}{\Omega_{\mathbf{k}'\alpha}} \right\rangle_{\frac{\mathbf{k}'}{|\mathbf{k}'|}}.$$

In the previous notation both quantities  $P_{\mathbf{k}\alpha\beta}$  and  $\Delta_{\mathbf{k}\alpha\beta}$  are antisymmetric  $2 \times 2$  matrices. For the s-wave superconductor the superconducting order parameter will take form:

$$\hat{\Delta} = \begin{pmatrix} 0 & \Delta \\ -\Delta & 0 \end{pmatrix} = \Delta i\sigma_y.$$

In case of a triplet pairing the order parameter is a vector in a spin space, making the same notation to take slightly different form:

$$\hat{\Delta} = \begin{pmatrix} -d_1 + id_2 & d_3 \\ d_3 & d_1 + id_2 \end{pmatrix}. \quad (2.19)$$

Quite often in the literature the triplet order parameter is represented as a vector rather than a  $2 \times 2$  matrix. As in the text and my calculations I will stick to matrix notation I want to represent the formula connecting  $\mathbf{d}(\mathbf{k})$  vector and matrix notation:

$$\hat{\Delta}(\mathbf{k}) = \sum_{\mu} d_{\mu}(\mathbf{k})(\sigma_{\mu}i\sigma_2). \quad (2.20)$$

### 2.3 Green's function formalism.

Let us consider a physical system represented by the following Hamiltonian:

$$H = H_0 + H^i$$

where  $H_0$  corresponds to free particles and  $H^i$  to their interaction. Thus, we can define system's density operator allowing to calculate expectation values of the system in equilibrium:

$$\langle \hat{A} \rangle = \frac{\text{Tr} [\hat{\rho}_H \hat{A}]}{\text{Tr} [\hat{\rho}_H]}, \quad \hat{\rho}_H = \frac{e^{-\beta(H-\mu N)}}{\text{Tr} [e^{-\beta(H-\mu N)}]}, \quad \beta = \frac{1}{k_B T}$$

then, if one wants to describe non-equilibrium state a total Hamiltonian is considered:

$$\mathcal{H}(t) = H + H'(t),$$

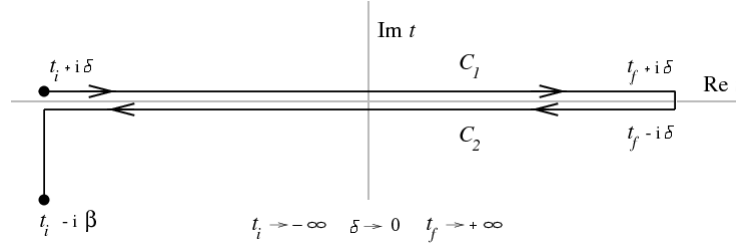
where  $H'(t)$  is perturbation of a system which is switched-on/off adiabatically at  $t = \mp\infty$ . Then the observable operator  $A$  average will be calculated with new wave-fucntions of the total Hamiltonian  $\mathcal{H}(t)$ .

$$\begin{aligned} \langle A \rangle &= \text{Tr} [\hat{\rho}_{\mathcal{H}(t)} \hat{A}] = \text{Tr} \left[ e^{-i \frac{\int \mathcal{H}'(t) dt}{\hbar}} \hat{\rho}_H e^{i \frac{\int \mathcal{H}'(t) dt}{\hbar}} \hat{A} \right] = \text{Tr} [\hat{\rho}_H \hat{A}_{\mathcal{H}}(t)], \\ \hat{A}_{\mathcal{H}} &= e^{i \frac{\int \mathcal{H}'(t) dt}{\hbar}} A e^{-i \frac{\int \mathcal{H}'(t) dt}{\hbar}} \end{aligned}$$

where  $\hat{A}_{\mathcal{H}}(t)$  stands for the Heisenberg representation of operator  $\hat{A}$  of an observable quantity. The last thing needed before we could introduce contour ordered Green's function is a contour ordering operator. Let's assume we have two time-dependent operators and we have chosen two points on the time contour  $t$  and  $t'$ , then the contour ordering operator will act on these two operators in the following way:

$$T(A(t)B(t')) = \begin{cases} \hat{A}(t)\hat{B}(t'), & t >_c t' \\ -\hat{B}(t')\hat{A}(t), & t <_c t' \end{cases}$$

where  $t >_c t'$  that  $t$  is further along the contour than  $t'$ . Here we would use time ordering along contour known as Keldysh path and it is depicted on the picture:



**Figure 2.2:** Graphical representation of the Keldysh contour.

The Keldysh path starts at  $t_i$  with infinitely small imaginary elevation  $\delta$  above real axis, then proceeds to a time  $t_f$  where it crosses to lower half-plane and continues until reaching point corresponding to  $t_i$  from another side of the real axis where it goes down by the value of  $i\beta$ . This contour selection allows to disregard initial correlations while calculating averages. In general, it has been shown that assuming Keldysh path ordering of operators allows using techniques developed for equilibrium systems in non-equilibrium case. Now we can define contour ordered Green's function, for simplicity of notations all space and time coordinates are denoted as  $r = \{t, \dots, x^i, \dots\}$  where  $x^i$  defines position of  $i$ -th particle of the system:

$$G(r, r') = -i \langle T_k(\psi_{\mathcal{H}}(r) \psi_{\mathcal{H}}^{\dagger}(r')) \rangle \quad (2.21)$$

using this definition by adding additional subscript denoting a part of Keldysh contour  $C_{1,2}$  at which time coordinate is taken  $r_{1,2}$  one can introduce a Green function specified by Keldysh



contour:

$$\underline{G} = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix},$$

writing out for each of the components:

$$\begin{aligned} G_{11} &= G(r_1, r'_1) = G^{T_k}(r, r') = -i\langle T_k(\psi_{\mathcal{H}}(r_1)\psi_{\mathcal{H}}^\dagger(r'_1)) \rangle, \\ G_{12} &= G(r_1, r'_2) = G^<(r, r') = i\langle \psi_{\mathcal{H}}^\dagger(r'_2)\psi_{\mathcal{H}}(r_1) \rangle, \\ G_{21} &= G(r_2, r'_1) = G^>(r', r) = -i\langle \psi_{\mathcal{H}}(r'_1)\psi_{\mathcal{H}}^\dagger(r_2) \rangle, \\ G_{22} &= G(r_2, r'_2) = G^{\tilde{T}_k}(r, r') = -i\langle \tilde{T}_k(\psi_{\mathcal{H}}(r_2)\psi_{\mathcal{H}}^\dagger(r'_2)) \rangle, \end{aligned}$$

where  $\tilde{T}$  stands for reverse time ordering operator and can be obtained by reversing inequalities on time variables in definition of  $T$ . Upon consideration one can notice following relations between these functions:

$$\begin{aligned} G^{T_k}(r, r') &= -i\Theta(t - t')G^>(r', r) + i\Theta(t' - t)G^<(r, r'), \\ G^{\tilde{T}_k}(r, r') &= \Theta(t - t')G^>(r', r) + \Theta(t' - t)G^<(r, r'), \\ G^{T_k} + G^{\tilde{T}_k} &= G^> + G^< \end{aligned}$$

which in turn means that the four components are not linearly independent and there could be found a linear combination of them forcing one of the components to zero. By performing a rotation considered by Larkin and Ovchinnikov [35] one gets following form of a Green's function:

$$\begin{aligned} \underline{G} &= \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix} \\ G^R(r, r') &= \Theta(t - t')(G^>(r, r') - G^<(r, r')), \\ G^A(r, r') &= -\Theta(t' - t)(G^>(r, r') - G^<(r, r')), \\ G^K(r, r') &= G^>(r, r') + G^<(r, r') \end{aligned}$$

To consider electron system one needs to take into account an additional variable which is the spin of the electron. Then, instead of a  $\psi$  function one needs to plug in spinor in the definition of a Green's function (2.21) making a resulting function a  $4 \times 4$  matrix.

## 2.4 Dyson equation.

Let us start with the derivation of a motion equation for free electron Green's function. To do so consider the free electron Hamiltonian in second quantization representation:

$$\mathcal{H}^0(t) = \mathcal{H} - H^i = \sum_{\alpha\beta} \epsilon_{\alpha\beta}^0(t) \psi_{\alpha}^{\dagger} \psi_{\beta},$$

then one can calculate the time evolution of annihilation operator:

$$\frac{d\psi_{\iota}(t)}{dt} = \frac{i}{\hbar} [\mathcal{H}^0(t), \psi_{\iota}(t)] = -\frac{i}{\hbar} \sum_{\beta} \epsilon_{\iota\beta}^0(t) \psi_{\beta}(t),$$

and plug it in time ordered product will give us an equation of motion of a free electron Green's function:

$$\sum_{\iota} \left( i\delta_{\alpha\iota} \frac{\partial}{\partial t} - \epsilon_{\alpha\iota}^0(t) \right) \underline{G}_{\iota\beta}^0(r, r') = \delta_{\alpha\beta} \delta_K(t - t'),$$

where  $\delta_K$  stands as Dirac delta for time variable ordered on Keldysh contour. Now let us consider how Green's function equation of motion changes if a perturbation potential is introduced to Hamiltonian:

$$\mathcal{H}^v(t) = \sum_{\alpha\beta} \epsilon_{\alpha\beta}^0(t) \psi_{\alpha}^{\dagger} \psi_{\beta} + \sum_{\alpha\beta} v_{\alpha\beta}(t) \psi_{\alpha}^{\dagger} \psi_{\beta},$$

consequently Green's function equation of motion for new Hamiltonian can be written as:

$$\sum_{\iota} \left( i\delta_{\alpha\iota} \frac{\partial}{\partial t} - \epsilon_{\alpha\iota}^0(t) \right) \underline{G}_{\iota\beta}(r, r') = \delta_{\alpha\beta} \delta_K(t - t') + \sum_{\iota} v_{\alpha\iota}(t) \underline{G}_{\iota\beta}(r, r'), \quad (2.22)$$

but similar to Schroedinger equation, it might be too hard to obtain eigen-energies and eigen-functions of perturbed state making is impossible to obtain Green's function  $G$  by definition (2.21). Using the same approach as perturbation theory, one can construct perturbed Green's function as a perturbation series of unperturbed one  $G^0$ :

$$\begin{aligned} \underline{G}_{\alpha\beta}(r, r') &= \underline{G}_{\alpha\beta}^0(r, r') + \int_K dr'' \sum_{\iota\lambda} \underline{G}_{\alpha\iota}^0(r, r'') v_{\iota\lambda}(t'') \underline{G}_{\lambda\beta}^0(r'', r') + \\ &+ \int_K dr'' \int_K dr''' \sum_{\iota\lambda} \sum_{\iota'\lambda'} \underline{G}_{\alpha\iota}^0(r, r'') v_{\iota\lambda}(t'') \underline{G}_{\lambda\iota'}^0(r'', r''') v_{\iota'\lambda'}(t''') \underline{G}_{\lambda'\beta}^0(r''', r') + \dots \end{aligned}$$

where  $int_K$  means that integration variables are ordered on Keldysh contour. As one could easily see this expansion could be brought to a more compact form:

$$\underline{G}_{\alpha\beta}(r, r') = \underline{G}^0_{\alpha\beta}(r, r') + \int_K dr'' \sum_{\iota\lambda} \underline{G}^0_{\alpha\iota}(r, r'') v_{\iota\lambda}(t'') \underline{G}_{\lambda\beta}(r'', r'), \quad (2.23)$$

and one can check by substitution that the Green's function satisfying this relation also satisfies (2.22). Also with the same observation one can derive a conjugate form of Dyson equation:

$$\underline{G}_{\alpha\beta}(r, r') = \underline{G}^0_{\alpha\beta}(r, r') + \int_K dr'' \sum_{\iota\lambda} \underline{G}_{\alpha\iota}(r, r'') v_{\iota\lambda}(t'') \underline{G}^0_{\lambda\beta}(r'', r'). \quad (2.24)$$

Obtained equation is in fact, Dyson equation for single particle Green's function. In case of a superconductors one would need to include particle interaction part of Hamiltonian which in case of BCS theory would require consideration of two particle Green's function. Luckily, if system considered on a Keldysh contour it allows for application of Wick's theorem that states that many particle Green's function is in fact sum of one particle Green's functions products taken with a sign accounting for interchanging properties of the particles (important in case of fermions). As a result, particle interactions can be reduced to the average potential of all particles acting on one resulting in perturbation close to considered in derivation above, however full derivation allows to determine a new quantity via Dyson equations called self-energies:

$$\begin{aligned} \underline{G} &= \underline{G}^0 + \underline{G}^0 \otimes \underline{\Sigma} \otimes \underline{G}, \\ \underline{G} &= \underline{G}^0 + \underline{G} \otimes \underline{\Sigma} \otimes \underline{G}^0, \end{aligned} \quad (2.25)$$

where similarly to Keldysh Green's function self-energy consists of retarded, advanced and Keldysh parts:

$$\underline{\Sigma} = \begin{pmatrix} \Sigma^R & \Sigma^K \\ 0 & \Sigma^A \end{pmatrix}, \quad (2.26)$$

and  $\otimes$  symbol means conventional multiplication of matrices and convolution over a time variable.

## 2.5 Quasiclassical Green's function. Eilenberger equation.

Dyson equation contains a full description of the system, however solution to that equation contains excessive information about systems behaviour on length and energy scales beyond limits of the interest. When one considers a superconducting system first such limit is that we restrict our consideration to an interval of a few superconducting gaps below and above Fermi energy. The second limit is that momentum of quasiparticles as we know from BCS theory is restricted to a thin layer within a Fermi sphere resulting in slow spatial variation of solution obtained in quasiclassical description. First, let's rewrite both Dyson equations (2.25) in slightly different form:

$$\begin{aligned}\underline{G}^{0-1} \otimes \underline{G} &= \underline{1}\delta(t-t') + \underline{\Sigma} \otimes \underline{G}, \\ \underline{G} \otimes \underline{G}^{0-1} &= \underline{1}\delta(t-t') + \underline{G} \otimes \underline{\Sigma}\end{aligned}$$

here, we defined an inverse operator  $\underline{G}^{0-1}$  which is essentially an operator of a differential equation to which  $\underline{G}^0$  is a solution, holding relation:

$$\underline{G}^{0-1} \otimes \underline{G}^0 = \underline{1}\delta(t-t').$$

By subtracting the two Dyson equations, one obtains following:

$$\underline{G}^{0-1} \otimes \underline{G} - \underline{G} \otimes \underline{G}^{0-1} = \underline{\Sigma} \otimes \underline{G} - \underline{G} \otimes \underline{\Sigma} \quad (2.27)$$

In order to change previously defined Green's function  $\underline{G}$  and self-energies  $\underline{\Sigma}$  to their quasiclassical form we need to perform two step procedure. First, we will shift to "centre of mass" reference frame or as it is also called Wigner representation. In order to do so we need to shift from the  $\{r, r'\} = \{t, \mathbf{x}, t', \mathbf{x}'\}$  set of coordinates to a new one  $\{\frac{t-t'}{2}, \frac{t+t'}{2}, \frac{\mathbf{x}-\mathbf{x}'}{2}, \frac{\mathbf{x}+\mathbf{x}'}{2}\}$  and then taking the Fourier transform for both "difference" coordinates one would arrive to following

set  $\{\hat{\mathbf{p}}, \mathbf{R} = \frac{\mathbf{x}+\mathbf{x}'}{2}, E, t = \frac{t+t'}{2}\}$ . With moving to that coordinate set also meaning of  $\otimes$  changes:

$$(A \otimes B)(r, r') = \int d\mathbf{x}'' \int_{-\infty}^{\infty} dt'' A(r, r'') B(r'', r')$$

$$(A \odot B)(\mathbf{p}, \mathbf{R}, E, t) = e^{\frac{i\hbar}{2}(\nabla_{\mathbf{p}'} \nabla_{\mathbf{R}''} - \nabla_{\mathbf{p}''} \nabla_{\mathbf{R}'} + \partial_{E''} \partial_{t'} - \partial_{E'} \partial_{t''})} A(\mathbf{p}'', \mathbf{R}'', E'', t'') B(\mathbf{p}', \mathbf{R}', E', t') \quad \text{for,}$$

$$(\mathbf{p}', \mathbf{R}', E', t') = (\mathbf{p}'', \mathbf{R}'', E'', t'') = (\mathbf{p}, \mathbf{R}, E, t).$$

then operator  $\underline{G}^{0-1}$  in the Wigner representation will take form:

$$\underline{G}^{0-1} = \underline{E} - \xi(\mathbf{p}), \quad \underline{E} = \begin{pmatrix} \epsilon^R \tau_3 & 0 \\ 0 & \epsilon^A \tau_3 \end{pmatrix}, \quad \xi(\mathbf{p}) = \hbar(v)_F(\mathbf{k} - \mathbf{k}_F).$$

Let's now calculate commutator on the right-hand side of (2.27) using definition of  $\odot$ :

$$\begin{aligned} \underline{G}^{0-1} \odot \underline{G} - \underline{G} \odot \underline{G}^{0-1} &= \underline{E} \odot \underline{G} - \underline{G} \odot \underline{E} - \xi(\mathbf{p}) \odot \underline{G} + \underline{G} \odot \xi(\mathbf{p}) = \\ &= \underline{E} \odot \underline{G} - \underline{G} \odot \underline{E} - \xi(\mathbf{p}) \underline{G} + \frac{i\hbar}{2} \nabla_{\mathbf{p}} \xi(\mathbf{p}) \nabla_{\mathbf{R}} \underline{G} + \underline{G} \xi(\mathbf{p}) + \frac{i\hbar}{2} \nabla_{\mathbf{p}} \xi(\mathbf{p}) \nabla_{\mathbf{R}} \underline{G} + \dots \approx \\ &\approx \underline{E} \odot \underline{G} - \underline{G} \odot \underline{E} + i\hbar \mathbf{v}(\mathbf{p}) \nabla_{\mathbf{R}} \underline{G}, \end{aligned}$$

where higher order gradient terms were neglected due to us limiting our consideration to slowly varying functions. Then our previous equation (2.27) will transform into:

$$[\underline{E} - \Sigma, \underline{G}]_{\odot} + i\hbar \mathbf{v}(\mathbf{p}) \nabla_{\mathbf{R}} \underline{G} = 0, \quad [A, B]_{\odot} = A \odot B - B \odot A. \quad (2.28)$$

The second step would be to average functions in the Wigner representation over quasiparticle energy to eliminate dependence on the magnitude of the momentum but keep the dependence of the momentum direction. Thus a quasiclassical Green's function is introduced:

$$\underline{g}(\mathbf{R}, E, t) = \frac{i}{\pi} \int_{-\infty}^{\infty} d\xi(p) \underline{G}(\mathbf{p}, \mathbf{R}, E, t).$$

Such definition contains a flaw: Green's function  $\underline{G}$  behaviour at high energies is proportional to  $1/\xi$  making integral diverge, but as has been told before we are interested in system's behaviour in the vicinity of Fermi energy so a cutoff can be introduced as discussed by Serene and Rainer [36], or by following diagrammatic expansion of Eilenberger [30]. Then the Eilenberger

equation for quasiclassical Green's function will read:

$$[\underline{E} - \underline{\sigma}, \underline{g}]_{\odot} + i\hbar v_F \nabla_{\mathbf{R}} \underline{g} = 0. \quad (2.29)$$

Writing it down for each of the components of Green's function will hold:

$$\begin{aligned} i\hbar v_F \nabla_{\mathbf{R}} g^R + [\epsilon^R \tau_3 - \sigma^R, g^R]_{\odot} &= 0, \\ i\hbar v_F \nabla_{\mathbf{R}} g^A + [\epsilon^A \tau_3 - \sigma^A, g^A]_{\odot} &= 0, \\ i\hbar v_F \nabla_{\mathbf{R}} g^K + (\epsilon^R \tau_3 - \sigma^R) \odot g^K - g^K \odot (\epsilon^A \tau_3 - \sigma^A) + g^R \odot \sigma^K - \sigma^K \odot g^A &= 0, \end{aligned}$$

where components of  $\underline{\sigma}$  defined in the following way:

$$\sigma^{R,A} = \begin{pmatrix} \Sigma^{R,A} & \Delta^{R,A} \\ \tilde{\Delta}^{R,A} & \tilde{\Sigma}^{R,A} \end{pmatrix}, \quad \sigma^K = \begin{pmatrix} \Sigma^K & \Delta^K \\ -\tilde{\Delta}^K & -\tilde{\Sigma}^K \end{pmatrix}$$

where  $\sim$  means the symmetry relation between two functions:  $\tilde{\Phi}(\mathbf{p}, \mathbf{R}, E, t) = \Phi^*(-\mathbf{p}, \mathbf{R}, -E^*, t)$  which physically stands for particle-hole symmetry. With respect to that symmetry the quasiclassical Green's functions  $g^R, g^A$  and  $g^K$  can be shown to have the form similar to  $\sigma^{R,A,K}$ :

$$g^{R,A} = \begin{pmatrix} g^{R,A} & f^{R,A} \\ \tilde{f}^{R,A} & \tilde{g}^{R,A} \end{pmatrix}, \quad g^K = \begin{pmatrix} g^K & f^K \\ -\tilde{f}^K & -\tilde{g}^K \end{pmatrix}. \quad (2.30)$$

These functions allow to obtain a very important quantity *momentum resolved* local density of states (LDOS):

$$N(\mathbf{p}, \mathbf{R}, E) = -\frac{1}{2\pi} \text{Im} \left( \text{Tr} [g^R(\mathbf{p}, \mathbf{R}, E)] \right), \quad (2.31)$$

and as a quantity observed in the experiment *total* local density of states:

$$N(\mathbf{R}, E) = \frac{\int_{FS} \frac{d^2 \mathbf{p}'_F N(\mathbf{p}, \mathbf{R}, E)}{(2\pi)^3 |v_f(\mathbf{p}'_F)|}}{\int_{FS} \frac{d^2 \mathbf{p}'_F}{(2\pi)^3 |v_f(\mathbf{p}'_F)|}}, \quad (2.32)$$

where  $\int_{FS}$  means integral over the Fermi surface. In case of the  $^3\text{He}$  these expressions simplify considerably and will be used further in the simplified form. The second quantity is more commonly used and can be directly measured in the experiment, while first quantity is less

commonly used but gives an insight into the behaviour of the bound states.

### 2.5.1 Order parameter. Gap equation.

In BCS theory order parameter defined as a mean-field of Cooper pairs acting on a quasiparticle. It is worth noting that in quasiclassics the average  $\langle b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}'\beta} \rangle_T$  is by definition  $f^K$  from 2.30. That allows to directly adapt the formula 2.18 for the quasiclassical Green's function formalism:

$$\Delta_{i,j}(\mathbf{p}, \mathbf{R}, t) = \int \frac{d\Omega_{\mathbf{p}'}}{4\pi} V(\mathbf{p}, \mathbf{p}') \int_{-E_c}^{E_c} \frac{dE}{2i\pi} f_{i,j}^K(\mathbf{p}', \mathbf{R}, E, t), \quad (2.33)$$

where we defined an  $i, j$  component of  $2 \times 2$  matrix  $\Delta$ . When, someone talks about different kinds of pairing in superconductor they consider the decomposition of quasiparticle interaction potential over basis of functions corresponding to the full symmetry group of the normal state of the system. This means that in a case of superfluid  $^3\text{He}$  a following decomposition is considered:

$$V(\mathbf{p}, \mathbf{p}') = \sum_{l=0}^{\infty} (2l+1) V_l(p, p') P_l(\mathbf{p} \cdot \mathbf{p}'),$$

where  $P_l$  is Legendre polynomials. For p-wave pairing  $V_1(p, p')$  turns out to be the biggest coefficient, without any loss of precision this quantity is assumed to be constant in the considered energy interval. Substituting this in (2.33) holds following expression for triplet order-parameter:

$$\Delta_{i,j}(\mathbf{p}, \mathbf{R}, t) = \int \frac{d\Omega_{\mathbf{p}'}}{4\pi} 3V_t(\mathbf{p} \cdot \mathbf{p}') \int_{-E_c}^{E_c} \frac{dE}{2i\pi} f_{i,j}^K(\mathbf{p}', \mathbf{R}, E, t), \quad (2.34)$$

which is called self-consistent gap equation.

## 2.6 Projector operators. Riccati parametrization.

Together with quasiclassical Green's function normalization condition and Gap equation Eilenberger equation make a self-consistent system of equations that is sufficient to describe a superconducting system. Eilenberger excluded quasiparticle energy from variables of the equation, allowing us not to consider high energy perturbations. The obtained equation is fairly easy to solve and allowed to consider problems that were thought as too hard to solve with Dyson equation. On the other side, it turns out that Eilenberger equation is numerically unstable,

meaning that even a slight deviation from the normalized initial condition will explode exponentially along the solution's trajectory, making it really tedious if approached numerically. Because of that, there were attempts to parametrise equation in such a way that it will allow producing some numerical results [37]. In this section, I will follow [38] as a clear example of the derivation of what is known as Riccati parametrisation. First, let's start with the Green's function normalization condition:

$$\underline{g} \odot \underline{g} = -\pi^2 \underline{1}. \quad (2.35)$$

This condition is essential in determining if obtained solution is physical. It allows to construct a quantity called projector that will automatically satisfy (2.35):

$$\underline{P}_{\pm} = \frac{1}{2} \left( \underline{1} \mp \frac{1}{i\pi} \underline{g} \right).$$

It is easy to check that projectors defined this way will have following properties:

$$\begin{aligned} \underline{P}_+ + \underline{P}_- &= \underline{1}, \\ \underline{P}_{\pm} \odot \underline{P}_{\pm} &= \underline{P}_{\pm}, \\ \underline{P}_{\pm} \odot \underline{P}_{\mp} &= 0. \end{aligned}$$

The quasiclassical Green's function can be expressed via projector operators in the following ways:

$$\underline{g} = -i\pi(2\underline{P}_+ - \underline{1}) = -i\pi(\underline{1} - 2\underline{P}_-) = -i\pi(\underline{P}_+ - \underline{P}_-).$$

Using last expression and a fact that Eilenberger equation is linear, one can obtain following equations of motion for projector operators:

$$[\underline{E} - \underline{\sigma}, \underline{P}_{\pm}] \odot - i\hbar v_F \nabla_{\mathbf{R}} \underline{P}_{\pm} = 0.$$

Keldysh part of a green's function obeys relation  $\underline{g}^R \odot \underline{g}^K + \underline{g}^K \odot \underline{g}^A = 0$ . This implies equalities  $\underline{P}_{\pm}^R \underline{g}^K \underline{P}_{\pm}^A = -\underline{g}^K \underline{P}_{\mp}^A = -\underline{P}_{\mp}^R \underline{g}^K$  which allows to make a proper parametrisation of  $\underline{g}^K$ :

$$\underline{g}^K = -2i\pi \left( \underline{P}_+^R \odot \underline{X}^K \underline{P} \odot \underline{P}_-^A + \underline{P}_-^R \odot \underline{X}^K \underline{P} \odot \underline{P}_+^A \right),$$



where  $X^K$  and  $Y^K$  matrices parametrizing  $g^k$  which should obey same symmetry relations as  $\underline{g}$ . When substituted into the quasiclassical equation for Keldysh component:

$$((E^R - \mu)\tau_3 - \sigma^R) \odot g^K - g^K \odot ((E^A - \mu)\tau_3 - \sigma^A) + i\hbar v_F \nabla_{\mathbf{R}} g^K + g^R \odot \sigma^K - \sigma^K \odot g^A = 0,$$

one obtains equations on the parameters:

$$\begin{aligned} P_+^R \odot [((E^R - \mu)\tau_3 - \sigma^R) \odot X^K - X^K \odot ((E^A - \mu)\tau_3 - \sigma^A) + \sigma^K + i\hbar v_F \nabla_{\mathbf{R}} X^K] \odot P_-^A &= 0, \\ P_-^R \odot [((E^R - \mu)\tau_3 - \sigma^R) \odot Y^K - Y^K \odot ((E^A - \mu)\tau_3 - \sigma^A) - \sigma^K + i\hbar v_F \nabla_{\mathbf{R}} Y^K] \odot P_+^A &= 0. \end{aligned} \quad (2.36)$$

Projectors  $P_{\pm}^{R,A}$  themselves can be parametrised by multitude of the different ways. We choose a particular parametrisation of projector operators by  $\gamma^{R,A}, \tilde{\gamma}^{R,A}$  which would result in the simplest form of equations on those parameters. One can easily check that following parametrisation satisfies all projector's properties:

$$\begin{aligned} P_+^R &= \begin{pmatrix} 1 \\ -\tilde{\gamma}^R \end{pmatrix} \odot (1 - \gamma^R \odot \tilde{\gamma}^R)^{-1} \odot (1, \gamma^R), \\ P_-^R &= \begin{pmatrix} -\gamma^R \\ 1 \end{pmatrix} \odot (1 - \tilde{\gamma}^R \odot \gamma^R)^{-1} \odot (\tilde{\gamma}^R, 1), \end{aligned}$$

Expression for advanced projectors can be obtained by considering the connection between advanced and retarded parts of Green's function  $g^A = \tau_3 g^R \tau_3$ . Applying this to projectors we obtain:

$$\begin{aligned} P_+^A &= \begin{pmatrix} -\gamma^A \\ 1 \end{pmatrix} \odot (1 - \tilde{\gamma}^A \odot \gamma^A)^{-1} \odot (\tilde{\gamma}^A, 1), \\ P_-^A &= \begin{pmatrix} 1 \\ -\tilde{\gamma}^A \end{pmatrix} \odot (1 - \gamma^A \odot \tilde{\gamma}^A)^{-1} \odot (1, \gamma^A). \end{aligned}$$

Now, once substituted in Eilenberger equation one obtains equations of motion for  $\gamma^{R,A}$  and  $\tilde{\gamma}^{R,A}$ :

$$\begin{aligned}
 i\hbar v_F \nabla_{\mathbf{R}} \gamma^{R,A} + (\epsilon^{R,A} \odot \gamma^{R,A} + \gamma^{R,A} \odot \epsilon^{R,A}) &= \gamma^{R,A} \odot \tilde{\Delta}^{R,A} \odot \gamma^{R,A} + \\
 &+ \left( \Sigma^{R,A} \odot \gamma^{R,A} - \gamma^{R,A} \odot \tilde{\Sigma}^{R,A} \right) - \Delta^{R,A}, \\
 i\hbar v_F \nabla_{\mathbf{R}} \tilde{\gamma}^{R,A} - (\epsilon^{R,A} \odot \tilde{\gamma}^{R,A} + \tilde{\gamma}^{R,A} \odot \epsilon^{R,A}) &= \tilde{\gamma}^{R,A} \odot \Delta^{R,A} \odot \tilde{\gamma}^{R,A} + \\
 &+ \left( \tilde{\Sigma}^{R,A} \odot \tilde{\gamma}^{R,A} - \tilde{\gamma}^{R,A} \odot \Sigma^{R,A} \right) - \tilde{\Delta}^{R,A}
 \end{aligned} \tag{2.37}$$

Afterwards it is useful to consider following form of  $X^K$  and  $Y^K$ :

$$X^K = \begin{pmatrix} x^K & 0 \\ 0 & 0 \end{pmatrix}, \quad Y^K = \begin{pmatrix} 0 & 0 \\ 0 & \tilde{x}^K \end{pmatrix}.$$

Substituting them into (2.36) will hold:

$$\begin{aligned}
 i\hbar v_F \nabla_{\mathbf{R}} x^K + (\epsilon^R \odot x^K - x^K \odot \epsilon^A) + \left( -\gamma^R \odot \tilde{\Delta}^R - \Sigma^R \right) \odot x^K + x^K \odot \left( -\tilde{\Delta}^A \odot \gamma^A + \Sigma^A \right) &= \\
 &= -\gamma^R \odot \tilde{\Sigma}^K \odot \tilde{\gamma}^A + \Delta^K \odot \tilde{\gamma}^A + \gamma^R \odot \tilde{\Delta}^K - \Sigma^K, \\
 i\hbar v_F \nabla_{\mathbf{R}} \tilde{x}^K - (\epsilon^R \odot \tilde{x}^K - \tilde{x}^K \odot \epsilon^A) + \left( -\tilde{\gamma}^R \odot \tilde{\Delta}^R - \tilde{\Sigma}^R \right) \odot \tilde{x}^K + \tilde{x}^K \odot \left( -\tilde{\Delta}^A \odot \gamma^A + \tilde{\Sigma}^A \right) &= \\
 &= -\tilde{\gamma}^R \odot \tilde{\Sigma}^K \odot \gamma^A + \tilde{\Delta}^K \odot \gamma^A + \tilde{\gamma}^R \odot \Delta^K - \tilde{\Sigma}^K.
 \end{aligned} \tag{2.38}$$

It is possible to consider different forms of  $X^K$  and  $Y^K$  for example, as it has been done by Shelakov [1980 JETP]:

$$X^K = \begin{pmatrix} F & 0 \\ 0 & F \end{pmatrix}, \quad Y^K = \begin{pmatrix} \tilde{F} & 0 \\ 0 & \tilde{F} \end{pmatrix}.$$

The advantage of this parametrization is that the equilibrium solution for functions  $F$  will hold  $F = \tanh(\frac{\epsilon}{2k_B T}) = -\tilde{F}$ , which is convenient for perturbation expansion from equilibrium. However, chosen parametrisation allows for a more symmetric form of the equation which is one of the goals of this parametrization. As we see obtained equations (2.37,2.38) are not linear any more, but these type of equations and their solutions are well studied. This enables us to use

all of the uncovered properties of such equations for our investigations [39]. To summarize the results of the parametrisation we would express the components of the quasiclassical Green's function in terms of  $\gamma^{R,A}$ ,  $\tilde{\gamma}^{R,A}$  and  $x^K, \tilde{x}^K$ :

$$\begin{aligned} g^{R,A} &= \mp i\pi N^{R,A} \odot \begin{pmatrix} 1 + \gamma^{R,A} \odot \tilde{\gamma}^{R,A} & 2\gamma^{R,A} \\ -2\tilde{\gamma}^{R,A} & -1 - \tilde{\gamma}^{R,A} \odot \gamma^{R,A} \end{pmatrix}, \\ g^K &= -2i\pi N^K \odot \begin{pmatrix} x^K - \gamma^R \odot \tilde{x}^K \odot \tilde{\gamma}^A & -\gamma^R \odot \tilde{x}^K + x^K \odot \gamma^A \\ -\tilde{\gamma}^R \odot x^K + \tilde{x}^K \odot \tilde{\gamma}^A & \tilde{x}^K - \tilde{\gamma}^R \odot x^K \odot \gamma^A \end{pmatrix} \odot N^A, \\ N^{R,A} &= \begin{pmatrix} (1 - \gamma^{R,A} \odot \tilde{\gamma}^{R,A})^{-1} & 0 \\ 0 & (1 - \tilde{\gamma}^{R,A} \odot \gamma^{R,A})^{-1} \end{pmatrix}, \end{aligned}$$

here in the first line minus sign corresponds to the parametrisation of the retarded component of the Green's function and plus sign stands for the advanced.

For further illustration of Ricatti equation properties I will move to the dimensionless notation via following procedure. I will consider this procedure for one of the equations in (2.37) as it is identical to the rest of them. For equilibrium situation  $\odot$  operation turns into a matrix multiplication and will be considered further in that way. First, let us divide the whole equation by  $2\pi k_B T_c$ :

$$i \frac{\hbar v_f}{2\pi k_B T_c} \nabla \gamma - \gamma \frac{\tilde{\Delta}}{2\pi k_B T_c} \gamma + \frac{E}{2\pi k_B T_c} \gamma - \gamma \frac{\tilde{E}}{2\pi k_B T_c} + \frac{\Delta}{2\pi k_B T_c} = 0, \quad E = \epsilon - \Sigma, \quad \tilde{E} = -\epsilon - \tilde{\Sigma}$$

The first coefficient in the equation is superconductors coherence length it can be brought under differentiation sign allowing to consider spatial variable normalized by coherence length. All other quantities can be substituted by primed ones and considered to be represented in  $2\pi k_B T_c$  energy units. After all the manipulations equation would take form:

$$i \partial'_x \gamma - \gamma \tilde{\Delta}' \gamma + E' \gamma - \gamma \tilde{E}' + \Delta' = 0,$$

where  $\partial'_x$  denotes differentiation along quasiparticle's trajectory. Further, we presume that equation is written in natural dimensions and omit ' in the notation.

Solution of this equation  $\gamma(x)$  with initial condition  $\gamma(0) = \gamma_0$  can be associated with three

quantities  $U(x, \gamma(x)), V(x, \gamma(x)), W(x, \gamma(x))$  that obey following set of equations:

$$\begin{aligned} i\partial_x U(x) + (E - \gamma(x) \odot \tilde{\Delta}) \odot U(x) &= 0, \quad U(0) = 1, \\ i\partial_x V(x) + V(x)(-\tilde{E} - \tilde{\Delta}\gamma(x)) &= 0, \quad V(0) = 1, \\ i\partial_x W(x) + V(x)\tilde{\Delta}U(x) &= 0 \quad W(0) = 0. \end{aligned}$$

Now let's assume that we have a different initial condition  $\gamma_0^\dagger$  and we want to find a solution to the same equation  $\gamma^\dagger(x)$ . According to a theorem from [39] one could do that without solving the original equation. By knowing a solution  $\gamma(x)$  for initial condition  $\gamma_0$  with three additional functions  $U(x)$ ,  $V(x)$  and  $W(x)$  new solution  $\gamma^\dagger(x)$  can be obtained by the formula:

$$\gamma^\dagger(x) = \gamma(x) + U(x)\delta(1 + W(x)\delta)^{-1}V(x), \quad \delta = \gamma_0^\dagger - \gamma_0 \quad (2.39)$$

How can this formula be useful if we need to solve the actual equation? The answer is that we can find a particular solution which is easy to obtain: a homogeneous solution. Let us consider an equation where quantities  $\Delta$  and  $\tilde{\Delta}$  are independent of the coordinate  $\mathbf{R}$ :

$$-\gamma_h \tilde{\Delta} \gamma_h + E \gamma_h - \gamma_h \tilde{E} + \Delta = 0.$$

Later I will neglect diagonal self-energies making  $E = -\tilde{E}$  interchangeable with  $\gamma_h$ . Then one can consider a substitution  $\Gamma_h = \tilde{\gamma}_h$ :

$$-\Gamma_h^2 + 2 * E \Gamma_h + \tilde{\Delta} \Delta = 0,$$

with some additional definition of a matrix square root function one obtains a solution for  $\gamma_h$ :

$$\gamma_h = \tilde{\Delta}^{-1} \left( \sqrt{E^2 - \tilde{\Delta} \Delta} - E \right).$$

Also by straightforward calculation one can prove that  $\tilde{\Delta} \Delta = -|\Delta^2| \mathbb{1}$  reducing matrix square root operation to an algebraic square root and thus giving  $\gamma_h$ :

$$\gamma_h = \frac{1}{E \pm \sqrt{E^2 + |\Delta^2|}} \hat{\Delta},$$

where  $\hat{\Delta}$  is 2x2 matrix and thus denoted with hat. To summarize now we can build any solution for Riccati equation, knowing  $\gamma_h$  and the initial condition. As mentioned by Eilenberger [30] there is a problem of obtaining initial condition for quasiclassical equations. This problem should be solved for each case individually. In my case I approach it by stating periodicity of self-consistent solution. By starting with homogeneous solution I ensure that normalization condition is fulfilled as it fulfilled by any solution of Riccati equations (2.37,2.38) due to parametrization. With equations and their initial conditions defined we left with only one key feature to consider: boundary conditions.

## 2.7 Quasiclassical boundary conditions.

Many articles have shown that unusual compared to conventional superconductors dependence of order parameter  $\Delta$  on Cooper's pair momentum in  $^3\text{He}$  can lead to the emergence of bound states [16,20,22,24]. Usually articles show that the bound states emergence requires for the order parameter to change its sign as a spatial dependence. And while one can think of a "domain" regions of order parameter with walls between them on which bound states exist there is another possible realization of such situation. The sign change requirement is satisfied in the presence of a specular wall. As order parameter linearly depends on the momentum, the sign change of the momentum component perpendicular to the boundary due to the boundary scattering would change the sign of the order parameter. Thus allowing the existence of a bound state at the boundaries of the system.

However, describing a wall in quantum mechanics usually means constituting it with area of infinite potential emerging on an atomic scale. In other words, it is a strong inhomogeneity on a small scale and thus beyond quasiclassical theory reach. However, there is a way to work around that problem by deriving connection between "incoming" and "outgoing" propagators and applying them at the boundaries of the system.

Derivation itself can be done from the first principles [40] and holds an elegant answer in case of a specular boundaries. But for further consideration of magnetic boundaries we would require an approach that considers Riccati parametrisation [41]. For further discussion, we

will consider the following decomposition of a quasiclassical Green's function:

$$g^{R,A} = \mp 2i\pi \begin{pmatrix} \mathcal{G}^{R,A} & \mathcal{F}^{R,A} \\ -\tilde{\mathcal{F}}^{R,A} & -\tilde{\mathcal{G}}^{R,A} \end{pmatrix} \pm i\pi \begin{pmatrix} \tau_3 & 0 \\ 0 & \tau_3 \end{pmatrix}$$

$$g^K = -2i\pi \begin{pmatrix} \mathcal{X} & \mathcal{Y} \\ \tilde{\mathcal{Y}} & \tilde{\mathcal{X}} \end{pmatrix} = \begin{pmatrix} \mathcal{G}^R & \mathcal{F}^R \\ -\tilde{\mathcal{F}}^R & -\tilde{\mathcal{G}}^R \end{pmatrix} \odot \begin{pmatrix} x & 0 \\ 0 & \tilde{x} \end{pmatrix} \odot \begin{pmatrix} \mathcal{G}^A & \mathcal{F}^A \\ -\tilde{\mathcal{F}}^A & -\tilde{\mathcal{G}}^A \end{pmatrix}$$

where  $x, \tilde{x}$  satisfy equations (2.38) and  $\mathcal{G}^{R,A}, \mathcal{F}^{R,A}$  are given by corresponding coherence amplitudes:

$$\mathcal{G} = (1 - \gamma \odot \tilde{\gamma})^{-1}, \quad \mathcal{F} = (1 - \gamma \odot \tilde{\gamma})^{-1} \odot \gamma$$

$$\tilde{\mathcal{G}} = (1 - \tilde{\gamma} \odot \gamma)^{-1}, \quad \tilde{\mathcal{F}} = (1 - \tilde{\gamma} \odot \gamma)^{-1} \odot \tilde{\gamma}.$$

These quantities will also satisfy following equations which can be verified by direct substitution:

$$\begin{aligned} \mathcal{G} &= 1 + \mathcal{G} \odot \gamma \odot \tilde{\gamma}, & \mathcal{F} &= \gamma + \mathcal{F} \odot \tilde{\gamma} \odot \gamma \\ \tilde{\mathcal{G}} &= 1 + \tilde{\mathcal{G}} \odot \tilde{\gamma} \odot \gamma, & \tilde{\mathcal{F}} &= \tilde{\gamma} + \tilde{\mathcal{F}} \odot \gamma \odot \tilde{\gamma}. \end{aligned} \tag{2.40}$$

In order to derive boundary conditions I will follow a certain recipe. First, I would need to establish a connection between quasiclassical propagators and their variables corresponding to trajectories incoming and outgoing towards and from scattering region. Second, I will define scattering matrix that binds incoming and outgoing coherence and distribution functions. Scattering matrix itself is defined by normal state Bloch wave solutions as all scattering events are happening at the energies higher than superconducting gap and temperature of the considered system. Then boundary condition will result in mixing incoming and outgoing variables of quasiclassical propagators with  $S$  matrix corresponding to the normal state scattering solution. Further, I will restrict our consideration to the stationary case as a derivation of boundary conditions for Keldysh component is a bit more cumbersome and doesn't bring any benefit towards understanding of thesis final results.

To proceed with first step we divide all variables by projection of the group velocity on the Fermi momentum which has same sign for  $\gamma^R, \tilde{\gamma}^A$  and the opposite for  $\tilde{\gamma}^R, \gamma^A$ . In order to distinguish between incoming and outgoing trajectories we will use small letters for incoming

quantities  $\gamma^{R,A}$ ,  $\tilde{\gamma}^{R,A}$  and capital for outgoing  $\Gamma^{R,A}$ ,  $\tilde{\Gamma}^{R,A}$ . Then quasiclassical propagator for trajectories toward scatterer would depend on:

$$\underline{g} = \underline{g}(\gamma^R, \tilde{\Gamma}^R, \Gamma^A, \tilde{\gamma}^A),$$

and for outgoing trajectories:

$$\underline{g} = \underline{g}(\Gamma^R, \tilde{\gamma}^R, \gamma^A, \tilde{\Gamma}^A).$$

Normal state scattering matrices in particle-hole space take form:

$$\underline{S} = \begin{pmatrix} S & 0 \\ 0 & \tilde{S}^\dagger \end{pmatrix}, \quad \underline{S}^\dagger = \begin{pmatrix} S^\dagger & 0 \\ 0 & \tilde{S} \end{pmatrix}.$$

Each of these matrices corresponds to scattering event from momentum  $\mathbf{p}_F$  to momentum  $\mathbf{p}'_F$ . Due to particle-hole symmetries some of the incoming quantities  $\gamma^A, \tilde{\gamma}^R$  will have their momentum opposite towards their propagation. To note that explicitly we will also introduce notation where index  $k$  will denote all momenta pointing away from the scatterer and  $p$  for all momenta pointing towards it. As we would see further it is convenient for formulation to introduce following quantities:

$$\gamma'^R_{kk'} = \sum_p S^R_{kp} \gamma^R_p \tilde{S}^R_{pk'}, \quad \gamma'^A_{pp'} = \sum_k S^R_{pk} \gamma^A_k \tilde{S}^A_{kp'},$$

similarly for respective particle-hole conjugated quantities:

$$\tilde{\gamma}'^R_{pp'} = \sum_k \tilde{S}^R_{pk} \tilde{\gamma}^R_k S^R_{kp'}, \quad \tilde{\gamma}'^A_{kk'} = \sum_p \tilde{S}^R_{kp} \tilde{\gamma}^A_p S^A_{pk'}.$$

The anomalous functions  $\mathcal{F}^R$  are obtained from a sum over all virtual multiple Andreev scattering events that are accompanied by interface scattering. Let us start with consideration of retarded Green's function with directions  $k$  that are directed away from the scatterer:

$$g^R = g^R(\gamma^R, \tilde{\Gamma}^R).$$

Using the equations (2.40) we can introduce effective coherence functions on the interface as

solutions to:

$$\mathcal{F}_{kk'}^R = \gamma_{kk'}'^R + \sum_{k_1} \mathcal{F}_{kk_1}^R \odot \tilde{\gamma}_{k_1}^R \odot \gamma_{k_1 k'}'^R.$$

Since the only component in quasiclassical approximation that contributes to slowly varying envelope function for trajectory  $k$  is  $k' = k$  we obtain:

$$\mathcal{F}_k^R = \gamma_k^R \odot (1 - \tilde{\gamma}_k^R \odot \gamma_k'^R)^{-1}$$

Similarly, one defines  $\mathcal{G}^R$ :

$$\mathcal{G}^R = (1 - \gamma'^R \odot \tilde{\gamma}^R)^{-1} = 1 + \mathcal{F}^R \odot \tilde{\gamma}^R, \quad \mathcal{F}^R = \mathcal{G}^R \odot \gamma'^R$$

The same way obtained relation for particle-hole conjugates with result that  $\tilde{\mathcal{F}}^R = \tilde{\mathcal{G}}^R \odot \tilde{\gamma}'^R$ . But from equations (2.40) we know that  $\mathcal{F}$  obeys:

$$\mathcal{F}_k^R = \Gamma_k^R + \mathcal{F}_k^R \odot \tilde{\gamma}_k^R \odot \Gamma_k^R = \mathcal{G}_k^R \odot \Gamma_k^R$$

From this equation, one obtains a solution for outgoing trajectory:

$$\Gamma_k^R = (\mathcal{G}_k^R)^{-1} \odot \mathcal{F}_k^R,$$

where a more general quantity needed for further formulation of boundary conditions can be introduced:

$$\Gamma_{k \leftarrow k'}^R = (\mathcal{G}_k^R)^{-1} \odot \mathcal{F}_{kk'}^R. \quad (2.41)$$

Similarly, considering equations (2.40) and dependence of  $g^{R,A}$  from its variables, one obtains following equations for scattered coherence amplitudes:

$$\Gamma_k^R = \Gamma_{k \leftarrow k}^R, \quad \Gamma_p^A = \Gamma_{p \rightarrow p}^A, \quad \tilde{\Gamma}_p^R = \tilde{\Gamma}_{p \leftarrow p}^R, \quad \tilde{\Gamma}_k^A = \tilde{\Gamma}_{k \rightarrow k}^A. \quad (2.42)$$



The definition (2.41) can be rewritten in Dyson-like equation form:

$$\begin{aligned}
 \Gamma_{k \leftarrow k'}^R &= \gamma_{kk'}'^R + \sum_{k_1 \neq k} \Gamma_{k \leftarrow k_1}^R \odot \tilde{\gamma}_{k_1}^R \odot \gamma_{k_1 k'}'^R, \\
 \Gamma_{p' \rightarrow p}^A &= \gamma_{p'p}^A + \sum_{p_1 \neq p} \gamma_{p'p_1}^A \odot \tilde{\gamma}_{p_1}^A \odot \Gamma_{p_1 \rightarrow p}^A, \\
 \tilde{\Gamma}_{p \leftarrow p'}^R &= \tilde{\gamma}_{pp'}^R + \sum_{p_1 \neq p} \Gamma_{p \leftarrow p_1}^R \odot \gamma_{p_1}^R \odot \tilde{\gamma}_{p_1 p'}^R, \\
 \tilde{\Gamma}_{k' \rightarrow k}^A &= \tilde{\gamma}_{k'k}^A + \sum_{k_1 \neq k} \tilde{\gamma}_{k'k_1}^A \odot \gamma_{k_1}^A \odot \Gamma_{k_1 \rightarrow k}^A.
 \end{aligned} \tag{2.43}$$

From this equations we see that depending on the scatterer scattered coherence amplitude can depend on a few incoming amplitudes with different momenta and in general case one needs to solve a system of linear equations in order to determine scattered trajectories. However, in the case of specular boundary conditions when there is only one incoming and one outgoing trajectory for each momentum  $p$  a sum part in these equations turns to zero and we are left with a simpler form of the boundary conditions:

$$\Gamma_k^R = S \odot \gamma^R \odot \tilde{S}^\dagger, \quad \Gamma_p^A = S^\dagger \odot \gamma^A \odot \tilde{S}, \quad \tilde{\Gamma}_p^R = \tilde{S}^\dagger \odot \tilde{\gamma}^R \odot S, \quad \tilde{\Gamma}_k^A = \tilde{S} \odot \tilde{\gamma}^A \odot S^\dagger. \tag{2.44}$$

Now all that is left for complete formulation of boundary conditions is to determine a form of an  $S$  matrix. This is usually done by considering a normal state scattering matrix [42] which can be derived by straightforward calculation presented below.

Let us consider an interface between normal state ( $x < 0$ ) and a ferromagnetic layer ( $x > 0$ ). Because described phenomena emerge due to high-energy interactions it would be appropriate to assume that quasiparticle is described by the Bloch wave. Ferromagnetic layer is described as two bands, one for spin-down particles  $V_\downarrow$  and another for spin-up particles  $V_\uparrow = V_\downarrow - 2J$ , where  $\mathbf{J} = \mu \mathbf{B}_{eff}$  is an effective exchange field and  $\mu < 0$  is negative for solid  $^3He$  [43]. Lets consider the Bloch wave function of  $^3He$  atom:

$$\begin{aligned}
 \Psi_\sigma(x, \mathbf{r}_\parallel) &= \begin{cases} e^{i\mathbf{k}_\parallel \mathbf{r}_\parallel} (e^{ikx} + r_\sigma e^{-ikx}), & x < 0 \\ t_\sigma e^{i\mathbf{k}_\parallel \mathbf{r}_\parallel} e^{-\varkappa_\sigma x}, & x > 0 \end{cases} \\
 \hbar k(E) &= \sqrt{2mE - (\hbar k_\parallel)^2}, \quad \hbar \varkappa_\sigma(E) = \sqrt{2m(V_\sigma - E) - (\hbar k_\parallel)^2}
 \end{aligned}$$

After imposing continuity conditions on  $\Psi_\sigma(x, \mathbf{r}_\parallel)$  and its derivative, scattering matrix obtained:

$$S = \begin{pmatrix} e^{i\nu_\uparrow} & 0 \\ 0 & e^{i\nu_\downarrow} \end{pmatrix} = e^{i\frac{\nu_\uparrow + \nu_\downarrow}{2}} \begin{pmatrix} e^{i\nu} & 0 \\ 0 & e^{-i\nu} \end{pmatrix} \quad (2.45)$$

$$e^{i\nu_\sigma} = r_\sigma = \frac{k - i\chi_\sigma}{k + i\chi_\sigma}, \quad \nu = \frac{\nu_\uparrow - \nu_\downarrow}{2}$$

parameter  $\nu$  is well known in superconducting spintronics and is called "spin-mixing angle" [44] or "spin-dependent scattering phase shift".

The previous scattering matrix is obtained for Bloch wave being polarized in the direction of a magnetic layer. To generalize the formula let us see how scatters Bloch wave with spin polarized in direction  $m(\alpha, \phi)$ :

$$\left( \cos(0.5\alpha) e^{-i\frac{\phi}{2}} \uparrow_z + \sin(0.5\alpha) e^{i\frac{\phi}{2}} \downarrow_z \right) e^{i\mathbf{k}_\parallel \mathbf{r}_\parallel} e^{ikx},$$

after reflection, it will turn into:

$$\left( \cos(0.5\alpha) e^{-i\frac{\phi-\nu}{2}} \uparrow_z + \sin(0.5\alpha) e^{i\frac{\phi-\nu}{2}} \downarrow_z \right) e^{i\frac{\nu_\uparrow + \nu_\downarrow}{2}} e^{i\mathbf{k}_\parallel \mathbf{r}_\parallel} e^{-ikx}.$$

This means that scattering results in the precession of the scattered particle spin around the magnetization axis of the interface. Which leads to the generalized expression of the scattering matrix:

$$S = e^{i(\mathbf{m}\boldsymbol{\sigma})\frac{\nu}{2}} = \hat{1} \cos(0.5\nu) + i(\mathbf{m}\boldsymbol{\sigma}) \sin(0.5\nu) \quad (2.46)$$

where additional phase factor  $\frac{\nu_\uparrow + \nu_\downarrow}{2}$  is omitted as in quasiclassical description it won't be preserved.

Thus we have obtained all of the key components to describe  $3He$  in a compartment. We know how to treat this problem quasiclassically and which boundary conditions should be posed and the system boundaries. Also solving quasiclassical equations in Ricatti parametrizations self-consistently with Gap equation ensure adequate description of the system.

## Chapter 3

# Josephson current in p-wave superconductor.

The approach described in the previous chapter while being powerful in a capability of describing the system has a disadvantage of increasing its numerical difficulty when the dimensionality of the problem increases. Furthermore, for the problems with a relatively simple trajectory that approach would require to consider an infinite number of scatterings from the boundaries which is impossible to deal numerically without any additional assumptions. However, in the case when only order parameter spatial dependence is required another approach can be considered for problems with higher than one dimension and multiple-scattering trajectories. The approach is a minimization of a free energy functional. In order to do so, one should start with the Landau expansion of a free energy by the powers of the order parameter and add gradient terms in order to account for the order parameter spatial variation cost for the functional. The spatial variation would arise from the inconsistency of the stated boundary conditions with a bulk solution and gradient terms in the functional expansion.

### 3.1 Ginzburg-Landau functional.

Landau theory of second order phase transition postulates that in the described system a quantity  $\eta$  exists that can quantify how far away the system is from a symmetric state. This quantity should be equal zero in a state with higher symmetry and should take non-zero values in a lower symmetry state. Then the theory also postulates that any thermodynamic potential

should be an analytical function of that variable meaning that potentials can be expanded in powers of that quantity. Now let us assume that before the transition the system has a  $G_0$  symmetry group. Naturally, after the transition, our system will have a symmetry  $G$  which is a subgroup of  $G_0$ . Now from the group theory, one knows that any function could be represented as a linear combination of some functions  $\phi_1, \phi_2, \dots$  that transform into each other under group transformations. A choice of that functions is not unique and one can assemble them into subsets in such a way that functions in that subset transform into each other under all transformations in  $G_0$ . Matrices of these transformations that act on functions in the subsets are called irreducible representations of the group  $G_0$  and the functions are the basis of that representation. Which allows us to construct a quantity:

$$\tilde{\eta} = \sum_n \sum_i \alpha_i^{(n)} \phi_i^{(n)}$$

where  $n$  is an index of irreducible representation and  $i$  is an index of one of the representation's functions. Among all of the functions  $\phi_i^{(n)}$  there is always one that is invariant under all transformations of  $G_0$ . This means that this function has a symmetry  $G_0$  and we will denote it as  $\eta_0$ . Now, according to a definition of order parameter we should exclude  $\eta_0$  and consider as an order parameter only which is left of it:

$$\tilde{\eta} = \eta_0 + \eta, \quad \eta = \sum_n' \sum_i \alpha_i^{(n)} \phi_i^{(n)}.$$

A fact that functions  $\phi_1, \phi_2, \dots$  transform through themselves allows treating a change of order parameter as a change of coefficients  $\alpha_i^{(n)}$  rather than transformations of the functions  $\phi_i^{(n)}$  within their irreducible representation. Obviously, a thermodynamic potential should be independent of a choice of a coordinate system, it means that when order parameter changes under transformations of a group  $G_0$  thermodynamic potential should stay invariant:

$$\Phi(\eta_0 + \eta) = \Phi(\eta_0' + \eta').$$

Consequently, expansion of  $\Phi$  over the powers of order parameter  $\eta$  expressed in terms of  $\alpha_i^{(n)}$  should contain only invariant terms. As we consider  $\Phi$  being a function of  $\eta$  with  $\eta_0$  being fixed that excludes unitary function from our considerations and makes expansion terms to

be expressed in forms invariant to  $G_0$ . For functions in irreducible representation there is no linear invariant like that, otherwise, they would be reducible, but there is an invariant of a second order: positively determined quadratic form which can always be reduced to the sum of squares  $\alpha_i^{(n)}$ . Up to the second order precision functional would take the form:

$$\Phi = \Phi_0(P, T) + \sum_n ' A^{(n)}(P, T) \sum_i \alpha_i^{(n)2}.$$

At the transition point system should have symmetry  $G_0$  and it should also be a minimum of the functional  $\Phi$  with all  $\alpha_i^{(n)} = 0$ . That is satisfied when all  $A^{(n)}(P, T) \geq 0$ , while if one of the  $A^{(n)}(P, T)$  will change sign after the transition it will allow for the non-zero value of the order parameter to appear. Of course, it means that in the transition point on  $(P, T)$  diagram this coefficient should take zero value. This means that after a certain value of  $T$  all coefficients  $\alpha_i^{(n)}$  are zero while before that value coefficients corresponding to certain  $n$  would take non-zero values. In other words, a condition that phase transition will bring a more symmetric system to a less symmetric state will be satisfied with such expansion. During a phase transition only one of the functions  $A^{(n)}(P, T) \geq 0$  goes to 0 allowing for index  $n$  to be omitted. Then the order parameter of that phase will consist of functions that are in  $n$ th irreducible representation. Introducing denomination:

$$\alpha^2 = \sum_i \alpha_i^2, \quad \alpha_i = \alpha \omega_i, \quad \text{where} \quad \sum_i \omega_i^2 = 1,$$

which will turn our expansion in:

$$\Phi = \Phi_0(P, T) + \alpha^2 A(P, T) + \alpha^3 \sum_v C_v(P, T) f_v^{(3)}(\omega_i) + \alpha^4 \sum_v B_v(P, T) f_v^{(4)}(\omega_i) + \dots$$

where  $f_v^{(3)}(\omega_i), f_v^{(4)}(\omega_i) \dots$  are invariants of the corresponding order composed from  $\omega_i$  and sums over  $v$  contain as many terms as many independent invariants of corresponding order can be composed from  $\omega_i$ .

For our system to be stable at the transition point the potential should have a minimum for the value  $\alpha_i = 0$  meaning that third order terms should be zero while fourth order terms should be positive. We consider the situation when second order phase transition occurs over

a line on the  $(P, T)$  diagram rather than a set of isolated points it means that  $C_v(P, T) \equiv 0$  for any  $P$  and  $T$  which is equivalent to condition that it is impossible to construct a third order invariant out of  $\alpha_i$  quantities. This leads us to well known Ginzburg-Landau functional:

$$\Phi = \Phi_0(P, T) + \alpha^2 A(P, T) + \alpha^4 \sum_v B_v(P, T) f_v^{(4)}(\omega_i)$$

While this functional describes the homogeneous order parameter our interest lies within a spatial variation of such. If the order parameter will vary spatially then functional should depend on the order parameter derivatives. Knowing that functional should have a uniform solution, expansion over gradients  $\nabla \alpha_i$  should not contain first order terms, while 2nd order terms should be positive. As energy is determined as an integral over the whole space it means that any combination that gives the full derivative will give a constant that is not essential to determine a minimum. Consequently, all terms that proportional to derivatives of  $\alpha_i$  and all symmetrical combinations of  $\alpha_i \partial \alpha_k / \partial x$  can be omitted leaving only anti-symmetrical ones:

$$\alpha_i \frac{\partial \alpha_k}{\partial x} - \alpha_k \frac{\partial \alpha_i}{\partial x}.$$

## 3.2 Phases of superfluid $^3\text{He}$ .

Now one can move on to writing down a Ginzburg-Landau functional for  $^3\text{He}$ . In bulk state  $^3\text{He}$  have certain symmetries:

$$G_0 = U(1) \times SO(3)_S \times SO(3)_L \quad (3.1)$$

This implies that the order parameter should behave as a vector under both types of rotations in spin and orbital spaces. This is possible due to weak spin-orbit coupling in  $^3\text{He}$ . The quasiparticles that form the Cooper pairs in the  $^3\text{He}$  have effective mass way higher than the bare mass of  $^3\text{He}$  atom, which in turn allows independent rotation of orbital and spin components of the pair wave-function. Previously, this order parameter was defined as 2.19, but further I will explicitly extract the order parameter dependence from the quasiparticle momentum and consider it to be represented by a complex-valued function for each combination of  $\sigma_\alpha \cdot p_i$ . A mathematical object that follows this notation is a matrix, and as both spaces are three

dimensional our order parameter could be written as a  $3 \times 3$  matrix of complex values:

$$\mathbf{d} = \begin{matrix} & p_x & p_y & p_z \\ \begin{matrix} \sigma_X \\ \sigma_Y \\ \sigma_Z \end{matrix} & \begin{pmatrix} d_{Xx} & d_{Xy} & d_{Xz} \\ d_{Yx} & d_{Yy} & d_{Yz} \\ d_{Zx} & d_{Zy} & d_{Zz} \end{pmatrix} \end{matrix}.$$

Gauge invariance will be satisfied if the functional is expanded in terms of  $\mathbf{d}\mathbf{d}^*$ . Rotational invariance in spin and orbital spaces is guaranteed by contracting spin and momentum indices pairwise. The p-wave pairing order parameter is a complex  $3 \times 3$  matrix, there is only one second order term satisfying symmetry requirements but there exist several fourth order terms:

$$\begin{aligned} S &= \text{Tr}(\mathbf{d}\mathbf{d}^\dagger), \\ F_1 &= |\text{Tr}(\mathbf{d}\mathbf{d}^T)|^2, \quad F_2 = [\text{Tr}(\mathbf{d}\mathbf{d}^\dagger)]^2, \\ F_3 &= \text{Tr}[(\mathbf{d}\mathbf{d}^T)(\mathbf{d}\mathbf{d}^T)^*], \quad F_4 = \text{Tr}[(\mathbf{d}\mathbf{d}^\dagger)^2], \quad F_5 = \text{Tr}[(\mathbf{d}\mathbf{d}^\dagger)(\mathbf{d}\mathbf{d}^\dagger)^*], \end{aligned}$$

which will allow us to write down Ginzburg-Landau functional for the homogeneous order parameter:

$$\Phi = V(\Phi_0(P, T) + A(P, T)\text{Tr}(d\mathbf{d}^\dagger) + \sum_{v=1}^5 B_v(P, T)F_v((d))), \quad (3.2)$$

coefficients  $A(P, T)$  and  $B_v(P, T)$  can be obtained in the weak-coupling limit and will be as follows:

$$\begin{aligned} B_1(P, T) &= -\frac{1}{2}B_2(P, T) = -\frac{1}{2}B_3(P, T) = -\frac{1}{2}B_4(P, T) = \frac{1}{2}B_5(P, T) = B(P, T), \\ A(P, T) &= \frac{N_0(\frac{T}{T_c} - 1)}{3}, \quad B(P, T) = \frac{7\zeta(3)}{8} \frac{N_0}{60(\pi k_B T_c)^2}, \end{aligned} \quad (3.3)$$

where  $N_0$  is total number of the quasiparticles at zero temperature. From this functional one can derive Euler-Lagrange equations for extrema of the functional, but the equations obtained would be overdetermined and too complicated to solve. Instead, one could use group theory to present the systematic study of  $^3\text{He}$  phases. Such classification was first considered by Golo and Monastyrsky [45, 46] and Mineev [47]. In particular, Mineev identified all five main states that are obtained by factorization using continuous groups. A symmetry classification of  $G_0$

(3.1) allows for an explicit calculation of all bulk superfluid states with a remaining symmetry, i.e. states whose order parameter  $d_{\alpha,p}$  is invariant under a subgroup of  $G \subset G_0$ .

### 3.2.1 Continuous symmetries.

Every group element  $g \in G$  corresponds to a transformation, leaving  $\mathbf{d}$  invariant:

$$g\mathbf{d} = \mathbf{d}. \quad (3.4)$$

By introducing the generators of infinitesimal transformations  $\mathbf{J} = (J_x, J_y, J_z)$  of the group  $G$ ,  $g$  may be written as:

$$g = e^{-\frac{i}{\hbar}\boldsymbol{\theta} \cdot \mathbf{J}} \approx \mathbf{1} - \frac{i}{\hbar}\boldsymbol{\theta} \cdot \mathbf{J}$$

where  $\boldsymbol{\theta}$  is an arbitrary vector of infinitesimal length. Then equation (3.4) will take form:

$$(\boldsymbol{\theta} \cdot \mathbf{J})\mathbf{d} = 0, \quad \text{or} \quad J_i\mathbf{d} = 0, \quad i = x, y, z.$$

Order parameter  $d_{\alpha,p}$  components transforms like components of a vector in spin and orbital spaces respectively meaning that it could be expressed as a linear superposition of tensor products between unit vectors in orbital and spin spaces. As mentioned before the free energy functional is invariant under the symmetry group of the system. It implies that  $\mathbf{J}$  itself can be written as a linear combination of these transformation:

$$J_x = a_x S^x + b_x L^x,$$

$$J_y = a_y S^y + b_y L^y,$$

$$J_z = a_z S^z + b_z L^z + c\hat{\phi}.$$

Here  $\mathbf{S} = (S^x, S^y, S^z)$  and  $\mathbf{L} = (L^x, L^y, L^z)$  are respectively the spin and orbital angular-momentum operators in the 3D representation which are given by:

$$(S^\mu)_{\nu\lambda} = -i\hbar\epsilon_{\mu\nu\lambda},$$

$$(L^i)_{jk} = -i\hbar\epsilon_{ijk}.$$



Also,  $\hat{\phi} = -i\hbar\partial/\partial\phi$  is the operator for a gauge transformation. The form of the operator corresponds to the choice of the projection axis. Here, for the simplicity of the notation, it is chosen to coincide with z axis of the coordinate system. We have seven generators in total  $(\mathbf{S}, \mathbf{L}, \hat{\phi})$  with corresponding real parameters  $(\mathbf{a}, \mathbf{b}, c)$ . Now the equation (3.4) will yield:

$$a_i \sum_{\nu} \epsilon_{i\mu\nu} d_{\nu j} + b_i \sum_l \epsilon_{ijl} d_{\mu l} + i\delta_{iz} c d_{\mu j} = 0, \quad i = x, y, z. \quad (3.5)$$

These equations allow us to reduce a problem of possible phases of the system to a problem of finding non-trivial solutions of an overdetermined system of linear equations. Thus, leaving us with finding combinations of parameters  $(\mathbf{a}, \mathbf{b}, c)$  that will turn determinant of a corresponding system to zero.

First, I would like to start with the case where order parameter is invariant under all three rotations  $J_i$ ,  $i = x, y, z$  in both spin and momentum spaces. In that case non-trivial solution of (3.5) exists only if  $c = 0$  and all  $J_i$  transform as components of an angular momentum giving us condition  $|a_{\mu}| = |b_i| = 1$ .

1)  $c = 0$ ,  $|a_{\mu}| = |b_i| = 1$ . This order parameter preserves rotation symmetries in both spaces, and in this sense is most symmetric of all possible order parameters in consideration. By solving (3.5) one finds:

$$d_{\mu j} = \frac{\Delta_0}{\sqrt{3}} \delta_{\mu j},$$

which is a case of a more general form:

$$d_{\mu j} = \frac{\Delta_0}{\sqrt{3}} e^{i\phi} R_{\mu j}(\mathbf{n}, \theta) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where  $R_{\mu j}(\mathbf{n}, \theta)$  is a rotation matrix describing relative rotation of spin and orbital spaces. This state is the BW state, describing B phase. The explicit phase factor arises from broken gauge invariance. As general form of order parameter for this phase locks phase and relative rotation of spin to the orbital spaces, it not only brakes gauge invariance, but also group of relative rotations of spin and orbit spaces leaving only  $SO(3)_{S+L}$  symmetry. All other subgroups of  $G_0$  consist only from subgroups of  $U(1)$  it means that all other non-trivial solutions for  $d_{\mu j}$

will include symmetry along given axis, allowing us consider only  $i = z$  case in equation (3.5). The equation itself will then take a form:

$$a_z(\delta_{\mu 1}d_{2j} - \delta_{\mu 2}d_{1j}) + b_z(\delta_{j 1}d_{\mu 2} - \delta_{j 2}d_{\mu 1}) + icd_{\mu j} = 0. \quad (3.6)$$

This equation separates into four independent subsystems making the corresponding matrix of (3.6) block-diagonal. For  $d_{\mu j}$  to be non-zero determinant of the corresponding matrix should be equal zero:

$$\begin{aligned} D &= D_1 D_2 D_3 D_4 = 0, \\ D_1 &= ((a_z - b_z)^2 - c^2) ((a_z + b_z)^2 - c^2) \quad \text{for } d_{xx}, d_{xy}, d_{yx}, d_{yy}, \\ D_2 &= a_z^2 - c^2 \quad \text{for } d_{xz}, d_{yz}, \\ D_3 &= b_z^2 - c^2 \quad \text{for } d_{zx}, d_{zy}, \\ D_4 &= ic \quad \text{for } d_{zz}. \end{aligned}$$

2)  $c = 0, \forall a_z, b_z \in R$ . Which gives:

$$J_z = a_z S^z + b_z L^z,$$

allowing symmetry  $G = U(1)_{S_z} \times U(1)_{L_z}$  to remain. Because of  $D_1, D_2, D_3 \neq 0, D_4 = 0$  solution can be immediately obtained:

$$d_{\mu j} = e^{i\phi} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \Delta \end{pmatrix}.$$

This order parameter is still invariant under separate rotations around preferred directions in spin and orbital spaces. This phase is called the polar state.

3)  $c = a_z = 0, \forall b_z \in R$ . Which gives:

$$J_z = b_z L^z,$$

allowing only  $G = U(1)_{L_z}$  remaining symmetry. Because of  $D_1, D_3 \neq 0$  and  $D_2 = D_4 = 0$  the

order parameter has the structure:

$$d_{\mu j} = \Delta n_1 e^{i\phi} \begin{pmatrix} 0 & 0 & A \\ 0 & 0 & B \\ 0 & 0 & C \end{pmatrix},$$

with  $A, B$  and  $C$  being complex values and  $n_1 = (|A|^2 + |B|^2 + |C|^2)^{-\frac{1}{2}}$ . The condition  $a_z = 0$  implies that in this state a rotation symmetry with respect to spin space is completely broken. In this respect this state is more restrictive than planar phase, which is seen to be a special case with  $A = B = 0$ .

4)  $c = b_z = 0, \forall a_z \in R$ . Which gives:

$$J_z = b_z S^z,$$

allowing only  $G = U(1)_{S_z}$  remaining symmetry. It is similar to previous state with orbital and spin components interchanged:

$$d_{\mu j} = \Delta n_1 e^{i\phi} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ A & B & C \end{pmatrix}.$$

Here the rotational symmetry in orbital space is completely broken.

5)  $c = 0, a_z \pm b_z = 0$ . Which gives:

$$J_z = a_z (L^z \mp S^z),$$

with remaining symmetry  $G = U(1)_{S^z + L^z}$ . In this case  $D_1 = D_4 = 0$  and  $D_2, D_3 \neq 0$  which determines the form of the order parameter to be:

$$d_{\mu j} = \Delta n_2 e^{i\phi} \begin{pmatrix} A & B & 0 \\ \mp B & \pm A & 0 \\ 0 & 0 & C \end{pmatrix},$$

where  $A, B, C$  are complex numbers and  $n_2 = (2(|A|^2 + |B|^2) + |C|^2)^{-\frac{1}{2}}$ . Here the relative

symmetry  $U(1)_{L_z, S_z}$  with respect to rotation in spin and orbital spaces is broken.

This state is called  $\zeta$ -phase [48]. Form of the gap in orbital space is an ellipse and resembles a spherical gap of a B-phase. In fact, it represents precisely the order parameter structure of B<sub>2</sub>-phase which is the B-phase in an external magnetic field( with  $A = \frac{1}{2}(\Delta_{\uparrow\uparrow} + \Delta_{\downarrow\downarrow})$ ,  $B = -\frac{1}{2}(\Delta_{\uparrow\uparrow} - \Delta_{\downarrow\downarrow})$ ,  $C = \Delta_{\uparrow\downarrow}$ ). While if  $B = C = 0$  one obtains planar state. As it will be shown later this can be achieved by demanding some additional discrete symmetry from order parameter. Meaning that actual planar state contains both continuous and discrete symmetries.

6)  $b_z \mp c = 0, \forall a_z \in R$ . Which gives:

$$J_z = b_z(L^z \pm \phi) + a_z S^z,$$

giving remaining symmetry  $G = U(1)_{L_z \pm \phi} \times U(1)_{S_z}$ . In this case  $D_3 = 0$  and  $D_1, D_2, D_4 \neq 0$  which gives order parameter:

$$d_{\mu j} = \Delta \frac{e^{i\phi}}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & \mp i & 0 \end{pmatrix},$$

describing A-phase. Here invariance with respect to three dimensional rotations as well as the relative gauge-orbital symmetry  $U(1)_{L_z \pm \phi}$  is broken. Despite that, this phase is still invariant under rotations around one axis in spin space and joint transformation of the phase and a rotation around  $L_z$ .

7)  $b_z \mp c = 0, a_z = 0$ . Which gives:

$$J_z = b_z(L^z \pm \phi),$$

giving remaining symmetry  $G = U(1)_{L_z \pm \phi}$ . In this case  $D_1 = D_3 = 0$  and  $D_2, D_4 \neq 0$  which gives the order parameter:

$$d_{\mu j} = \Delta \frac{e^{i\phi} n_1}{\sqrt{2}} \begin{pmatrix} A & \mp iA & 0 \\ B & \mp iB & 0 \\ C & \mp iC & 0 \end{pmatrix}.$$

in addition to symmetries broken in previous case this state completely breaks spin rotation symmetry. Because of the more restrictive symmetry requirements, the order parameter is less symmetric than in A-phase. Parameters can be chosen in a special way:  $A = \frac{1}{2}(\Delta_{\uparrow} + \Delta_{\downarrow})$ ,  $B = \frac{1}{2}(\Delta_{\uparrow} - \Delta_{\downarrow})$ ,  $C = 0$ . Obtained form is a general form of  $A_2$ -phase order parameter which corresponds to an A-phase in a magnetic field.

8)  $a_z \mp c = 0, \forall b_z \in R$ . Which gives:

$$J_z = a_z(S^z \pm \phi) + b_z L^z,$$

giving remaining symmetry  $G = U(1)_{L_z} \times U(1)_{S_z \mp \phi}$ . In this case  $D_2 = 0$  and  $D_1, D_3, D_4 \neq 0$  which gives order parameter:

$$d_{\mu j} = \Delta \frac{e^{i\phi}}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & \mp i \\ 0 & 0 & 0 \end{pmatrix},$$

which is called  $\beta$  state. It is similar to ABM state where spin and orbital parts are interchanged. Accordingly, in this case a relative gauge-spin symmetry is broken.

9)  $a_z \mp c = 0, b_z = 0$ . Which gives:

$$J_z = a_z(S^z \pm \phi) + b_z L^z,$$

giving the remaining symmetry  $G = U(1)_{L_z} \times U(1)_{S_z \mp \phi}$ . In this case  $D_2 = 0$  and  $D_1, D_3, D_4 \neq 0$  which gives order parameter:

$$d_{\mu j} = \Delta \frac{n_1}{\sqrt{2}} \begin{pmatrix} A & B & C \\ \mp iA & \mp iB & \mp iC \\ 0 & 0 & 0 \end{pmatrix},$$

which is called  $\beta$  state. And it is similar to ABM state where spin and orbital parts are interchanged. Accordingly, in this case a relative gauge-spin symmetry is broken.

10)  $c = b_z \mp a_z$ . Which gives:

$$J_z = a_z(S^z \mp \phi) + b_z(L^z \pm \phi),$$

giving the remaining symmetry  $G = U(1)_{L_z \pm \phi} \times U(1)_{S_z \mp \phi}$ . In this case  $D_1 = 0$  and  $D_2, D_3, D_4 \neq 0$  which gives order parameter:

$$d_{\mu j} = \Delta \frac{1}{2} \begin{pmatrix} 1 & -i & 0 \\ \mp i & \mp 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

which is, again, a representation of  $A_1$  phase. In this case a  $U(1)$  symmetry that is a linear combination of all three symmetries is broken.

11)  $c \pm b_z = 0, c \pm a_z = 0$ . Which gives:

$$J_z = a_z(S^z + L^z \mp \phi),$$

giving the remaining symmetry  $G = U(1)_{L_z + S_z \mp \phi}$ . In this case  $D_2, D_3 = 0$  and  $D_1, D_4 \neq 0$  so that:

$$d_{\mu j} = \Delta \frac{n_3}{\sqrt{2}} \begin{pmatrix} 0 & 0 & A \\ 0 & 0 & \pm iA \\ B & \pm iB & 0 \end{pmatrix},$$

where  $A$  and  $B$  are complex and  $n_3 = (|A|^2 + |B|^2)^{-\frac{1}{2}}$ . This state is called  $\epsilon$  state and can be considered as a linear combination of  $A$  and  $\beta$  states. This state has relative gauge-spin and gauge-orbit symmetries broken.

12)  $2a_z \pm b_z = 0, c \pm' a_z = 0$ , . Which gives:

$$J_z = c(2L^z \mp S^z \pm' \phi),$$

giving the remaining symmetry  $G = U(1)_{(2L^z \mp S^z \pm' \phi)}$ . Because  $D_1, D_2 = 0$  and  $D_3, D_4 \neq 0$

one has:

$$d_{\mu j} = \Delta \frac{n_4}{\sqrt{2}} \begin{pmatrix} A & -iA & B \\ \mp iA & \mp A & \pm' iB \\ 0 & 0 & 0 \end{pmatrix},$$

where  $A$  and  $B$  are complex numbers and  $n_4 = (2|A|^2 + |B|^2)^{-\frac{1}{2}}$ . This state is a superposition of  $A_1$  and  $\beta$  states. Similarly to the previous case, it has two separate broken relative symmetries.

13)  $2b_z \pm a_z = 0$ ,  $c \pm b_z = 0$ , . Which gives:

$$J_z = c(2S^z \mp L^z \pm' \phi),$$

giving remaining symmetry  $G = U(1)_{(2S^z \mp L^z \pm' \phi)}$ . This is similar to (12) with spin and orbital parts interchanged.

Last two states are similar to case (11) because their symmetry groups  $G$  involves particular linear combinations of all three symmetries which are joint rotations. Consequently, their broken relative symmetries will be very similar.

Considering breaking of continuous symmetries we found 13 order parameter structures that still contain symmetry of a continuous subgroup  $G \subset G_0$ : one with remaining  $SO(3)$  symmetry, four with a  $U(1) \times U(1)$  and eight with remaining  $U(1)$  symmetry. Not all of this states are physical meaning they correspond to a functional minimum.

### 3.2.2 Discrete symmetries.

There is no reason why breaking of continuous symmetry should be preferred over discrete one. Similarly to the previous part we would consider restrictions imposed on the form of order parameter by generators of a discrete group, which will give us conditions on real valued parameters, which in turn will allow for a study of order parameter forms. A discrete groups are generated by a subset of elements meaning that each element can be written as a product of powers of generators.

Each element of  $G$  (3.1) can be written as a three rotations: a rotation in orbital space  $r^o$ , a rotation in spin space  $r^s$  and a gauge transformation  $e^{i\phi}$ . Clearly  $r^o$  and  $r^s$  should be elements of discrete subgroups of  $SO(3)$  and  $e^{i\phi}$  an element of a discrete subgroup of  $U(1)$ . The discrete subgroups of  $SO(3)$  and  $U(1)$  are well known. For  $SO(3)$  they are given by:

$C_n$  the rotations around z axis with angle  $2\pi k/n$  where  $k \in [1..n-1]$ . Elements of  $C_n$  are denoted as  $C_n^k$ ;

$D_n$  generated by  $C_n$  with an additional rotation by  $\pi$  around an orthogonal axis;

$T, O, Y$  the point groups of tetrahedron, cube and icosahedron respectively.

For each discrete subgroup  $G_d \in G_0$  there exists a minimal direct product subgroup  $G_o \times G_s \times G_\phi$  that contains  $G_d$ . It is natural to construct  $G_o, G_s$  and  $G_\phi$  by projecting  $G_d$  onto the factors  $SO(3)_L, SO(3)_S$  and  $U(1)$  of  $G$ . It also turns out that  $G_\phi$  is determined once  $G_o$  and  $G_s$  are given. So we will concentrate on constructing orbital and spin parts of  $G_d$ . There are normal subgroups  $G'_o$  and  $G'_s$  whose factor groups are isomorphic. Then group  $G_d$  is given by the set of all pairs of the elements of such isomorphic groups. As all invariant subgroups of  $SO(3) \times SO(3)$  are known, one can calculate the factor groups  $G_o/G'_o$  and  $G_s/G'_s$  which will give us all discrete subgroups of  $SO(3) \times SO(3)$ . Now we are able to determine the appropriate gauge transformation and form of the order parameter.

As the order parameter should be invariant under transformations of the discrete group  $G_d$  it leads to the system of equations:

$$r_k^s \mathbf{A}(r_k^o)^T e^{i\phi_k} = \mathbf{A},$$

which determines  $A_{\mu j}$  and  $\phi_k$  for given  $r_k^o, r_k^s$ . As this leads to a system of linear equations and variance of  $r_k^o, r_k^s$  leads to different solutions for  $A_{\mu j}$  describing the same phase I will concentrate only on solutions for  $\phi_k$  and phases that were not obtained with the help of continuous symmetry breaking. Solution for  $\phi_k$  will read:

$$|\phi_k| = \begin{cases} |\alpha_k \pm \beta_k| & \text{or,} \\ |\alpha_k| & \text{or,} \\ |\beta_k| & \text{or,} \\ 0 & \text{or,} \\ \pi, \end{cases}$$

where  $\alpha_k$  and  $\beta_k$  are rotation angles of  $r_k^o$  and  $r_k^s$ . Solutions for order parameter forms are



mainly repeat ones from the previous section, which means that these phases have also a discrete symmetry broken for them. Concentrating on phases not uncovered yet, we will come across:

- the planar state:

$$d_{\mu j} = \Delta \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

involving  $D_m$  symmetries for  $m > 1$ .

- the bipolar state:

$$d_{\mu j} = \Delta \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

with  $D_4$  symmetries involved.

- the  $\alpha$  state:

$$d_{\mu j} = \Delta \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\frac{\pi}{3}} & 0 \\ 0 & 0 & e^{i\frac{2\pi}{3}} \end{pmatrix},$$

with tetrahedral symmetries involved.

These are three main states together with other five from previous section which order parameter form is not obtained by linear combination or by choice of parameters of some other form. There is a possibility to study what kind of stationary point each of that state represents [49]. Once done that we would see that the three states that break the discrete symmetry (planar, bipolar,  $\alpha$  states) are saddle points of a free energy functional while the other five (B, A, A<sub>1</sub> polar,  $\beta$  states) correspond to local minima.

### 3.3 Boundary conditions.

After discussing how symmetries of the system shape form of the Ginzburg-Landau functional and particularly the order parameter we will move to the gradient terms. While the contribution of these terms clearly accounts for the order parameter spatial dependence, they also

allow formulating an important part of minimization problem: boundary conditions. I base my formulation of boundary conditions on variational principle. This approach was considered [50]. This approach allows to find boundary conditions for boundaries of various shapes and will be followed in this chapter.

I will start by writing down the expression for the gradient part of Ginzburg-Landau functional in Cartesian coordinates. As previously discussed the gradient term should contain only second order invariants of derivatives of order parameter with respect to the full symmetry of the system  $G_0$  excluding such combinations that give full derivative as such combinations are irrelevant in determining minima of the functional. With all that in mind the gradient part of Ginzburg-Landau functional would read:

$$\Phi_g = K_1(\partial_k d_{\alpha j} \partial_k d_{\alpha j}^*) + K_2(\partial_j d_{\alpha j} \partial_k d_{\alpha k}^*) + K_3(\partial_k d_{\alpha j} \partial_j d_{\alpha k}^*),$$

in a weak-coupling limit  $K_1 = K_2 = K_3 = K = \frac{3}{5} N_0 \xi_0^2$ . This expression can be written down in the covariant form which will hold for any choice of a coordinate system making further derivation valid in the general case. The covariant form of the expression will read:

$$\Phi_g = K_1(\mathbf{d}^*)_{\alpha j ; k} (\mathbf{d})^{\alpha j ; k} + K_2(\mathbf{d}^*)_{\alpha ; k}^k (\mathbf{d})^{\alpha j}_{; j} + K_3(\mathbf{d}^*)_{\alpha ; j}^k (\mathbf{d})^{\alpha j}_{; k},$$

where semicolon stands for covariant derivative of a tensor  $\mathbf{d}$ . Also with the help of Gauss theorem, one can perform a variation of a functional which with integration by parts will hold the following equation for surface terms:

$$\int dS_i (K_2 \mathbf{d})_{\alpha ; k}^j \delta_j^i + K_1 \mathbf{d}_{\alpha j}^{\cdot k} + K_3 (\mathbf{d})_{\alpha ; j}^k \delta (\mathbf{d}^*)^{\alpha j} = 0,$$

which after reducing it to components perpendicular and parallel to the outward surface normal will read:

$$\int dS_i (\mathbf{d}^*)^{\alpha k} (\delta_k^j - s^j s_k) (K_1 \mathbf{d})_{\alpha j}^{\cdot k} + K_3 (\mathbf{d})_{\alpha ; j}^k = 0,$$

which will lead to a known result that component of order parameter that depends on quasi-particle momentum normal to the surface should be zero  $s_i \mathbf{d}^{\alpha i} = 0$ . For components parallel to the boundary situation is a bit more tricky and usually depends on the choice of a coordinate

system.

If one considers the Cartesian coordinate system, then the boundary conditions for components parallel to the boundary (xy-plane) will read:

$$\partial_z \mathbf{d}_{\alpha,x} = 0, \quad \partial_z \mathbf{d}_{\alpha,y} = 0.$$

The case of the cylindrical coordinate system for a curved boundary of a radius  $r = R$  will differ. It can be shown that gradient terms, in that case, would consist of terms proportional to  $\frac{1}{r}$  and  $\frac{1}{r^2}$  and in the limit of  $r \gg \xi$  2nd order term can be neglected leading to the case similar to Cartesian coordinates in the opposite limit this term will dominate gradient part of the functional. Consequently, it will lead to a different formulation of a boundary condition:

$$\partial_r \mathbf{d}_{\alpha,\phi}|_{r=R} = \frac{1}{R} \mathbf{d}_{\alpha,\phi}|_{r=R}.$$

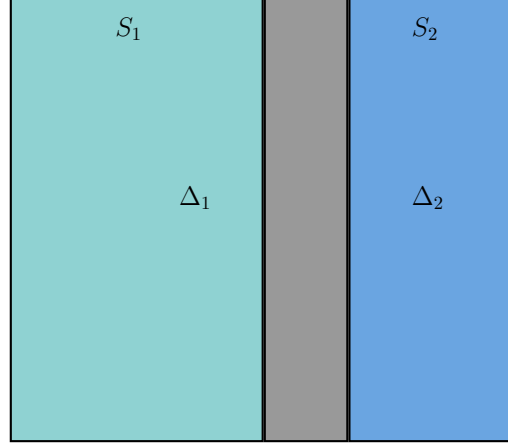
This boundary condition accounts for the local curvature of the boundary and allows to account for the physical condition that super current component perpendicular to the boundary should turn to zero at the boundary.

With the boundary conditions set I am now able to move to a minimization problem of Ginzburg-Landau functional. With a choice of a phase and shape of a boundary, I can obtain spatial dependence of the order parameter and discuss effects arising from the influence of the boundaries.

### 3.4 Josephson current in p-wave superfluid or superconductor

Previously it was shown that even for p-wave pairing condensate wave-function does not turn to zero at the boundary. In a general case of superconductivity, the condensate wave function is continuous. This means that the condensate wave function leaves a superconductor and there is a region  $l \approx \xi_0$  where it is not zero outside of a superconductor. This fact gives a rise to a basic case of an effect that I'm going to discuss in this chapter.

I will consider a system of two s-wave superconductors made from a same material near  $T_c$  separated by a thin layer of insulator  $l_d \ll \xi_0$  as shown on Fig.3.1. The wave functions of the superconductors "leak" into each other via a weak link making them wave-function of



**Figure 3.1:** Schematic representation of the Josephson junction with two s-wave superconductors separated by insulated layer.

the system's condensate with following boundary conditions needed to be satisfied at both boundaries:

$$\begin{aligned} \frac{\partial \psi_1}{\partial x} - \frac{2ie}{\hbar c} A_x \psi_1 &= \frac{\psi_2}{\lambda}, \\ \frac{\partial \psi_2}{\partial x} - \frac{2ie}{\hbar c} A_x \psi_2 &= \frac{\psi_1}{\lambda}. \end{aligned} \quad (3.7)$$

Here we consider wave-function after tunnelling to be  $\frac{1}{\lambda}$  proportional to the one of the bulk because of the condensate wave-function being small as system itself is close to  $T_c$ . Another thing needed is expression for super current in Ginzburg-Landau theory:

$$J = -\frac{ie\hbar}{2m} \left( \psi_1^* \frac{\partial \psi_1}{\partial x} - \psi_1 \frac{\partial \psi_1^*}{\partial x} \right) - \frac{2e^2}{mc} A_x \psi_1 \psi_1^*$$

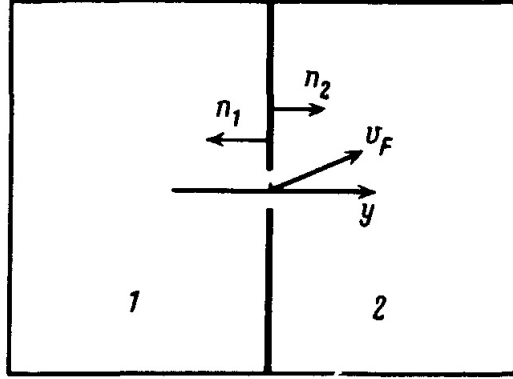
Combining super-current formula with boundary conditions (3.7) we will obtain an expression for Josephson current:

$$J_j = -\frac{ie\hbar}{2m\lambda} (\psi_1^* \psi_2 - \psi_1 \psi_2^*) \quad (3.8)$$

For a same type of metal difference between  $\psi_1$  and  $\psi_2$  is only in a phase factor  $e^{i\phi_{1,2}}$  which will transform our expression for  $j_J$  into:

$$J_j = \frac{e\hbar}{m\lambda} |\psi|^2 \sin(\phi_1 - \phi_2).$$

In case of a p-wave pairing not all phases have their  $U(1)$  symmetry completely broken while still having a different condensate wave-functions connected via weak link meaning that there is no definite phase factor that can be attributed to each case. This argument calls for a more accurate consideration of a problem with quasiclassical theory. This consideration was made by Kopnin [51] which derivation I'm going to follow here. The article considered the following setup 3.2.



**Figure 3.2:** Schematic representation of the Josephson junction for  $^3\text{He}$ .

The Eilenberger equation for  $^3\text{He}$  will take form:

$$-iv_F \nabla_{\mathbf{p}} f^{R,A}(E, \mathbf{p}, \mathbf{r}) - 2E f^{R,A}(E, \mathbf{p}, \mathbf{r}) + g^{R,A}(E, \mathbf{p}, \mathbf{r}) \Delta(\mathbf{p}) - \Delta(\mathbf{p}) g^{R,A}(E, \mathbf{p}, \mathbf{r}) = 0$$

where indexes  $R$  and  $A$  stand for retarded and advanced Green's functions and  $\mathbf{p}$  is a unit vector in direction of  $\mathbf{v}_F$ . Solution to the equation above can be obtained for temperatures near  $T_c$  if Green's function components will be expanded in terms of the order parameter and its derivatives. As we expand near  $T_c$  first term of the expansion should be sufficient. As there is no reflection of the quasi-particles at the weak link, then incoming solutions from region with  $\Delta_1$  should correspond to outgoing solutions from region with  $\Delta_2$ . All stated above would allow us to obtain solution approximations for incoming and outgoing trajectories on both

sides from the weak link:

$$\begin{aligned} f_i^R &= \frac{\Delta_1(\mathbf{p})}{E} - \frac{iv_f}{2E^2} \nabla_{\mathbf{p}} \Delta_1(\mathbf{p}), & f_o^R &= \frac{\Delta_2(\mathbf{p})}{E} - \frac{iv_f}{2E^2} \nabla_{\mathbf{p}} \Delta_2(\mathbf{p}), \\ f_o^R &= \frac{\Delta_2^*(\mathbf{p})}{E} + \frac{iv_f}{2E^2} \nabla_{\mathbf{p}} \Delta_2^*(\mathbf{p}), & f_i^R &= \frac{\Delta_1^*(\mathbf{p})}{E} + \frac{iv_f}{2E^2} \nabla_{\mathbf{p}} \Delta_1^*(\mathbf{p}), \end{aligned}$$

here subscripts i and o stand for incoming and outgoing solutions and advanced versions can be obtained by multiplying by  $-1$  and substituting  $\Delta_1 \leftrightarrow \Delta_2$ . Following Kopnin calculations we arrive to the formula for the Josephson current:

$$J_j = -i \frac{SN(0)mv_F\pi}{128T} \text{Tr} \left[ (\mathbf{d}_1^* \mathbf{d}_2 - \mathbf{d}_1 \mathbf{d}_2^*) + \frac{28\zeta(3)v_F}{15\pi^3 T} \left( \frac{\partial \mathbf{d}_1^*}{\partial n_1} \mathbf{d}_2 + \mathbf{d}_1^* \frac{\partial \mathbf{d}_2^*}{\partial n_2} - c.c. \right) + \frac{v_F^2}{144T^2} \left( \frac{\partial \mathbf{d}_1^*}{\partial n_1} \frac{\partial \mathbf{d}_2}{\partial n_2} - c.c. \right) \right],$$

where  $\partial/\partial n_i$  stands for the derivative along normal to the boundary and in case considered further will read:

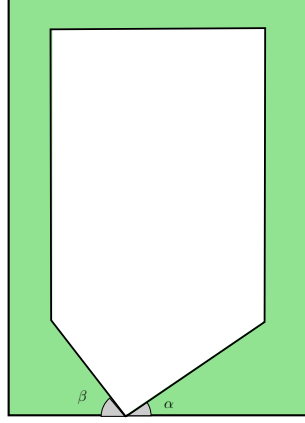
$$\begin{aligned} J_j &= -i \frac{SN(0)mv_F\pi}{128T} \left( 1 + \frac{56\zeta(3)v_F}{15\pi^3 T R_b} + \frac{v_F^2}{144T^2 R_b^2} \right) \text{Tr} [\mathbf{d}_1^* \mathbf{d}_2 - \mathbf{d}_1 \mathbf{d}_2^*] \approx \\ &\approx -i \frac{SN(0)mv_F\pi}{128T} \left( 1 + 0.45 \frac{\xi_0}{R_b} + 0.27 \frac{\xi_0^2}{R_b^2} \right) \text{Tr} [\mathbf{d}_1^* \mathbf{d}_2 - \mathbf{d}_1 \mathbf{d}_2^*], \end{aligned} \tag{3.9}$$

where  $R_b$  stands for boundary curvature.

### 3.5 P-wave Josephson junction modelling results.

Now with all the basic detail covered it is time to discuss the results. I consider a problem of a p-wave metal/ $^3\text{He}$  in confinement, which have different boundary geometry on each side of a weak link.

As we can see from the boundary conditions a single plane boundary acts as a filter on Cooper pairs in p-wave superconductors: it destroys pairs with perpendicular momentum components in its vicinity. That leads to the huge distortion in the p-wave order parameter near the boundary. Consequently, the aim of my calculation is to answer on how this distortion would affect the p-wave order parameter if the two boundaries intersect at given angle  $\alpha$ . Under the assumption that this distortion would be different for two different angles  $\alpha, \beta$  what would be a Josephson current emerging from the order parameter difference?



**Figure 3.3:** Experimental set-up scheme. The green area represents the area of a p-wave superconductor. The grey area is an area of a weak link appearing due to a close proximity of the two boundaries. Opening angles on the two sides of the weak link are parameters in that problem and are denoted as  $\alpha$  and  $\beta$ .

On the other hand, this effect is completely absent for the s-wave order parameter as the s-wave Cooper pair wavefunction is completely independent of the quasiparticle momentum. It allows to conclude that the calculated effect can be produced only in non-s-wave systems. If the effect magnitude will prove to be considerably large to be detected it could be a way to detect an unconventional pairing in the material.

Here I consider a set-up that depicted in a picture (Fig.3.3) where all the boundaries apart from wedges are considered to be far enough to not be of any significance. An important part of the set-up are wedges with characterising angles  $\alpha$  and  $\beta$  for right and left sides respectively. They are affecting order parameter in p-wave paired condensate in the vicinity of a weak link. According to intuition if two of these wedges with  $\alpha \neq \beta$  are brought in contact a supercurrent should flow while if opening angles are the same  $\alpha = \beta$  current should be equal to zero as order parameter is the same across a weak link. The present set-up also presumes that considered system is confined in the direction perpendicular to the picture's plane. Meaning that in the problem we focus on A phase solution structure and its spatial variation arising from boundary conditions.

As mentioned before calculation would concentrate on the area around a weak link as we presume that difference of the order parameters there forced by the boundaries will define the emerging effect. As we have seen from the boundary conditions component of the order parameter proportional to momentum normal to the boundary should go to zero while com-

ponent proportional to the tangential part of the momentum will have zero derivative. The geometry of the problem dictates the choice of a coordinate system to represent the order parameter and minimize the Ginzburg-Landau functional.

As previously mentioned the following matrix corresponds to the A-phase order parameter in Cartesian coordinates:

$$\mathbf{d} = \begin{matrix} & p_x & p_y & p_z \\ \begin{matrix} \sigma_X \\ \sigma_Y \\ \sigma_Z \end{matrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ d_{Zx} & d_{Zy} & 0 \end{pmatrix} \end{matrix}.$$

Now, if I want to switch to a reference system where the boundary conditions will take a simpler form for my geometry then it would be a cylindrical coordinate system. In this reference frame, we still can define our order parameter as  $3 \times 3$  matrix with columns corresponding to momenta along  $r, \phi$  and  $z$  axes.

$$\mathbf{d} = \begin{matrix} & p_r & p_\phi & p_z \\ \begin{matrix} \sigma_X \\ \sigma_Y \\ \sigma_Z \end{matrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ d_{Zr} & d_{Z\phi} & 0 \end{pmatrix} \end{matrix}.$$

Interchange of coordinate systems in orbital space should change only the representation of momentum dependence of the order parameter keeping the whole sum and thus the order parameter invariant. This gives the following connection between order parameter components of these two coordinate systems:

$$d_{Zx}(x, y) = d_{Zr}(r, \phi) \cos(\phi) - d_{Z\phi}(r, \phi) \sin(\phi), \quad d_{Zy}(x, y) = d_{Zr}(r, \phi) \sin(\phi) + d_{Z\phi}(r, \phi) \cos(\phi),$$

here primed letters denote cylindrical coordinate system while other correspond to the Cartesian one. This expression allows to write down a Ginzburg-Landau functional (3.2) including gradient terms:

$$\begin{aligned} \Phi[\Delta] = & \int_V dV \{ A(T)(|d_{Zr}|^2 + |d_{Z\phi}|^2) - 2B(|d_{Zr}|^2 + |d_{Z\phi}|^2)^2 - B(|d_{Zr}^2 + d_{Z\phi}^2|^2) + \\ & + K(|\frac{d_{Z\phi}}{r} - \frac{1}{r} \frac{\partial d_{Zr}}{\partial \phi} - \frac{\partial d_{Z\phi}}{\partial r}|^2 + |\frac{d_{Zr}}{r} + \frac{1}{r} \frac{\partial d_{Z\phi}}{\partial \phi} + \frac{\partial d_{Zr}}{\partial r}|^2 + 2|\frac{d_{Zr}}{r} + \frac{1}{r} \frac{\partial d_{Z\phi}}{\partial \phi}|^2 + 2|\frac{\partial d_{Zr}}{\partial r}|^2 \} \end{aligned}$$



where  $A, B$  and  $K$  coefficients that can be obtained from microscopic theory.

In calculation I do the order parameter minimization over a wedge area. The wedge area considered to have 'solid' boundaries on the inner curved boundary and on the straight sides of the wedge, while the outer edge is presumed to turn into a homogeneous solution, requiring for derivatives of order parameter components to vanish:

$$\frac{\partial d_{Zr}(r, \phi)}{\partial r} \Big|_{r=R_o} = 0, \quad \frac{\partial d_{Z\phi}(r, \phi)}{\partial r} \Big|_{r=R_o} = 0.$$

On the sides of an area boundary conditions will obey expression derived in the previous section: normal to the surface part of order parameter should go to zero while tangential component will have zero derivative in the direction of the boundary, making the normal component of the supercurrent vanish:

$$\frac{\partial d_{Zr}(r, \phi)}{\partial \phi} \Big|_{\phi=0, \alpha} = 0, \quad d_{Z\phi}(r, \phi) \Big|_{\phi=0, \alpha} = 0.$$

Last but not the least we have an inner boundary of our calculating area. It is intended to have it as close as possible to  $r = 0$  which is not advisable for a few reasons. First, is that Ginzburg-Landau theory deals with ranges bigger than a coherence length of a cooper pair  $\xi_0$  making any consideration pass that limit questionable. Second, if one revisits the form of a given functional (3.2) he will find that for  $r = 0$  gradient term in the integral diverges leaving us with an unsettling infinity under the integral sign. At this point boundary condition on a curved part of the boundary comes into play. For a curved boundary in the limit where curvature radius  $R_i \approx \xi_0$  we need to state a stronger boundary condition:

$$d_{Zr}(r, \phi) \Big|_{r=R_i} = 0, \quad \frac{\partial d_{Z\phi}(r, \phi)}{\partial r} \Big|_{r=R_i} = \frac{1}{R_i} d_{Z\phi}(R_i, \phi).$$

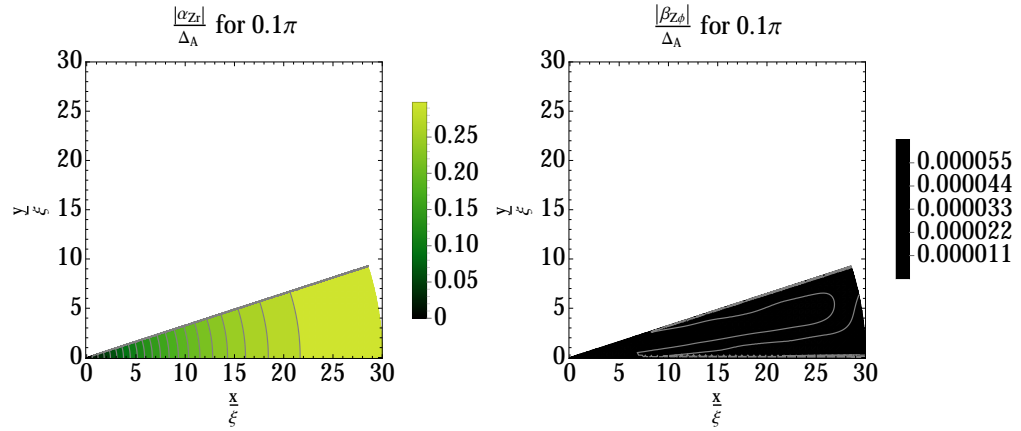
This condition ensures that tangential component at the boundary will be at least proportional to  $r$  making it impossible for the gradient term to diverge and as been mentioned before it ensures that the normal to the boundary component of the super current is zero.

From a numerical point of view, there is a small problem in the way these boundary conditions are stated. If one wants to minimize this functional numerically he would have to project his functions  $d_{Zr}(r, \phi)$  and  $d_{Z\phi}(r, \phi)$  on a grid. Then all derivatives are substituted

as some linear combinations of projected values of our functions, which would result for strict restrictions on that values combinations around the boundary. One can see, that corner points should obey two of that sort of equations, and satisfying one boundary condition does not guarantee automatic satisfaction of the other one. This requires to solve a system of linear equations to obtain a consistent equation on corner grid point values that would satisfy both boundary conditions. I will not go on the detailed derivation of such condition as it strongly depends on choice of derivative representation in the numerical scheme.

Minimization procedure was performed on a square grid in polar coordinates, allowing for better resolution in the region of interest while having a decent density of points in a region where the order parameter varies slightly. As calculation was performed over a large amount of "independent" variables  $\approx 10^6$  additional analytical expression for the gradient of a functional was required. While tedious the task was accomplished allowing for decent calculation time.

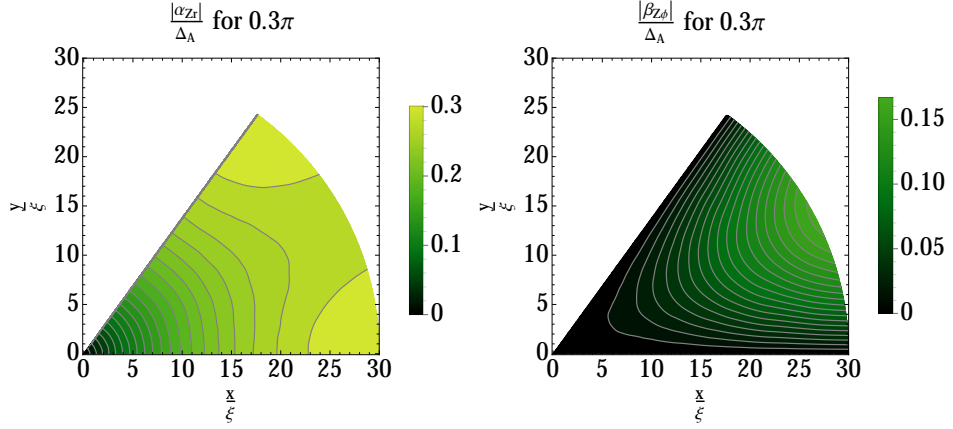
First, lets start with order parameter components spatial dependence for small angles:



**Figure 3.4:** The solution for  $\alpha = 0.1\pi$  obtained by minimisation of the Ginzburg-Landau functional.

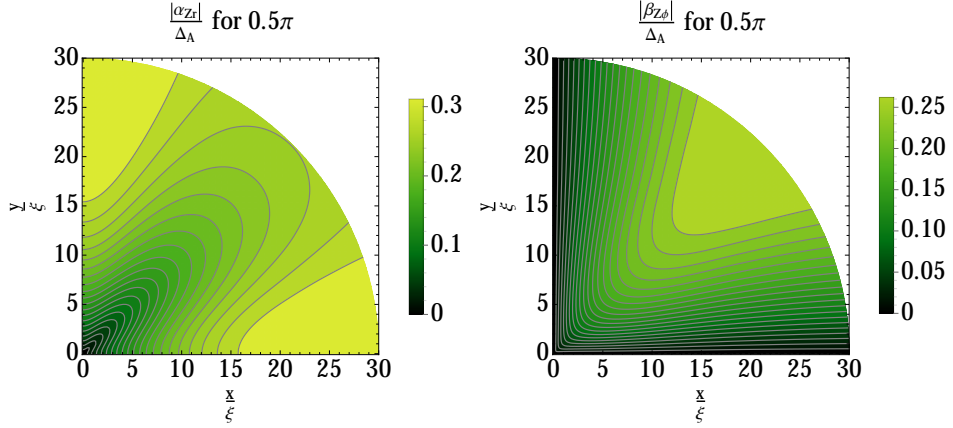
Because of two boundaries proximity, the normal component of the order parameter is being heavily suppressed while the other one quickly recovers over a length of  $\approx 10\xi_0$ . One can say that in that case, we obtain a polar phase. With the vanishing of the second component of order parameter relative phase between components is not determined. This allows "to restore" even a phase factor of a polar phase.

Moving to a wider wedge opening allows for the suppressed component to "breathe" within a confinement returning us to A phase with a spatial variation solution:



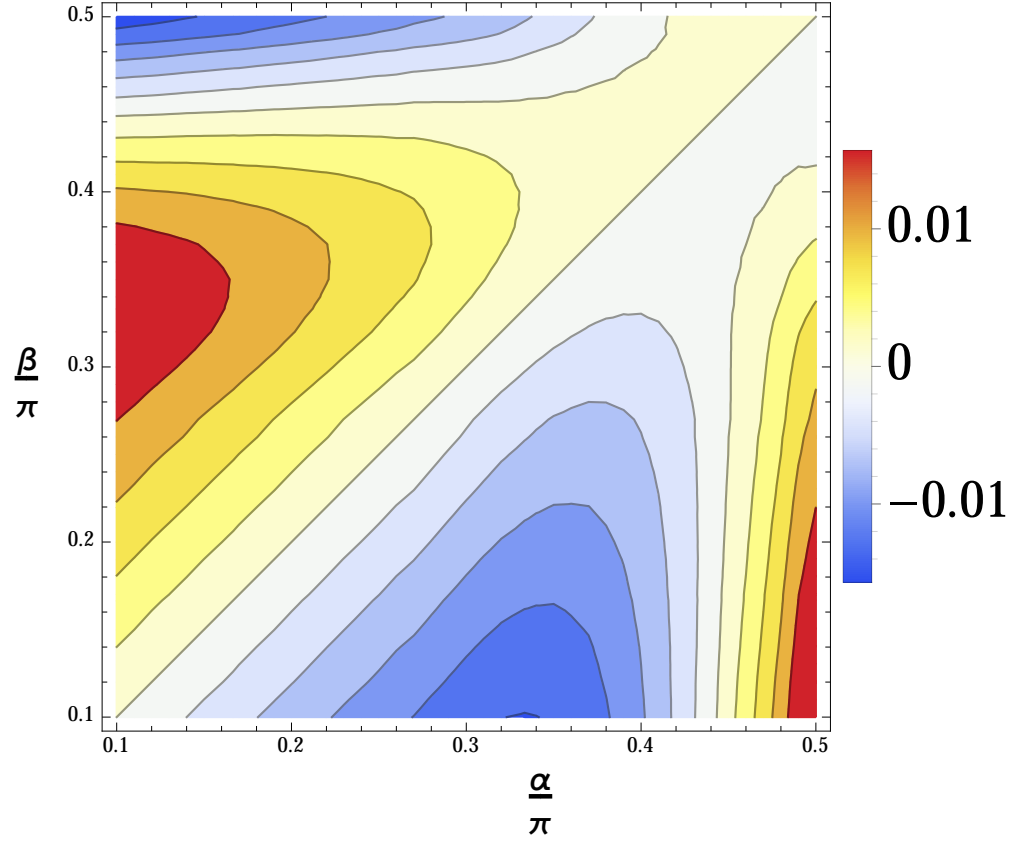
**Figure 3.5:** The solution for  $\alpha = 0.3\pi$  obtained by minimisation of the Ginzburg-Landau functional.

For the widest opening angle of  $\frac{\pi}{2}$  we could see that suppression takes place only along boundaries while in the middle suppressed order parameter component almost reaches to the value of an unsuppressed one:



**Figure 3.6:** The solution for  $\alpha = 0.5\pi$  obtained by minimisation of the Ginzburg-Landau functional.

After obtaining solutions for the set of angles on the right side we need to get it on the left side. This can be done by rotation of the original solution for each of the angles. As we know from the previous section A phase solution has a special relation between rotation in orbital space and gauge factor. This means that in order to obtain the bulk solution on the outer boundaries of both wedges the solution on the left should acquire the additional phase of  $e^{i\pi}$ . After these manipulations solutions from both sides can be plugged into formula (3.9) to obtain resulting magnitude and sign of Josephson effect:



**Figure 3.7:** Magnitude and direction of Josephson current in  $J/J_C$  units. Red colour stands for flow in the positive direction from  $\beta$  angle wedge to  $\alpha$  and blue for the opposite one.

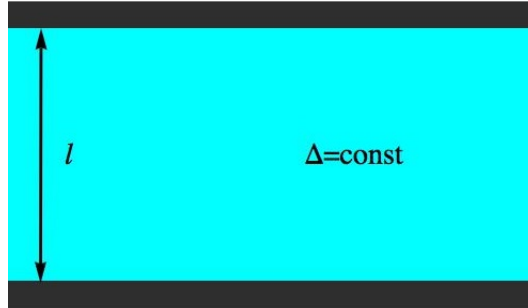
As we see the effect has a detectable magnitude as it is on the same order as the critical current of the system.

### 3.6 Discussion of the effect.

## Chapter 4

# Solution for Ricatti equation in 1D confinement.

I consider a problem of  $^3\text{He-B}$  being confined between two specular boundaries as it presented on the figure 4.1. In the presented case, the Green's function depends only on one coordinate. This makes the problem considered a good model problem because of the possibility of obtaining an analytical solution and developing a program to calculate it at the same time.



**Figure 4.1:** Scheme of the homogeneous solution case.  $^3\text{He}$  is represented by the blue colour. The smooth boundaries of the container are depicted by the dark grey colour.

As mentioned previously equations describing the problem are Ricatti equations and they have a special property that if you have a solution of that equation for one initial condition you can get it for any initial condition based on the formula (2.39).

It allows considering a problem in which zero energy states at the boundaries would exist analytically. It is a problem of a superfluid constrained in one direction between two specular

boundaries. In analytical consideration, I would neglect order parameter suppression that would occur between boundaries which will make considered order parameter to be bulk B-phase order parameter.

Considering 'specular' boundaries mean that a part of order parameter proportional to  $p_z$  changes its sign after each reflection. Solving that problem in quasiclassical approximation is identical to finding a solution for a quasiparticle moving through alternating potential. In this case, the solution should be periodical with a period of  $2L$  where  $L$  is the distance along the quasiparticle trajectory between two collisions with boundaries. For the case when the order parameter is a constant or can be divided into regions where it could be successfully approximated as a constant, solution of previous equations will give us:

$$\begin{aligned} U(\rho) &= e^{i(E-\gamma_h\tilde{\Delta})\rho}, \\ V(\rho) &= e^{i(-\tilde{E}-\tilde{\Delta}\gamma_h)\rho}, \\ W(\rho) &= e^{i(-\tilde{E}-\tilde{\Delta}\gamma_h)\rho} w e^{i(E-\gamma_h\tilde{\Delta})\rho} - w. \end{aligned}$$

For simplification of the notation I will introduce following quantities:

$$\begin{aligned} \Omega_1 &= E - \gamma_h\tilde{\Delta}, \\ \Omega_2 &= -\tilde{E} - \tilde{\Delta}\gamma_h, \end{aligned}$$

while  $w$  is defined as the solution of corresponding Sylvester equation:

$$\Omega_2 w + w \Omega_1 = \tilde{\Delta}. \quad (4.1)$$

Using those notations, formula of any solution of Ricatti equation (2.39) for the case of homogeneous order parameter will take form:

$$\gamma(\rho) = \gamma_h + e^{i\Omega_1\rho} \delta_i \frac{\hat{1}}{\hat{1} + (e^{i\Omega_2\rho} w e^{i\Omega_1\rho} - w) \delta_i} e^{i\Omega_2\rho}, \quad (4.2)$$

In considered problem order parameter is purely triplet making matrices  $\gamma_h\tilde{\Delta}$  and  $\tilde{\Delta}\gamma_h$  diagonal, also if self energies are neglected matrices  $E$  and  $\tilde{E}$  are diagonal as well, making

$\Omega_1 = \Omega_2 \equiv \Omega$  and being diagonal. Which allows to further simplify the formula:

$$\gamma(\rho) = \frac{\gamma(0)\Omega + i \tan(\rho\Omega)(E\gamma(0) + \Delta)}{\Omega - i \tan(\rho\Omega)(E - \gamma(0)\tilde{\Delta})} \quad (4.3)$$

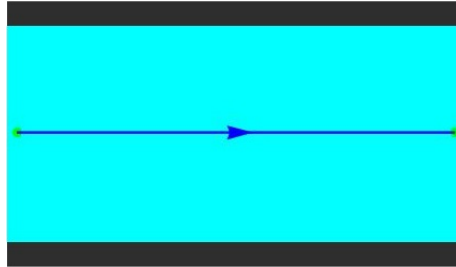
Let's use this formula to describe the gamma spatial dependence, quantities before the first reflection would be referred with index  $L$  quantities after -  $2L$ :

$$\begin{aligned} \gamma(L) &= \frac{\gamma(0)\Omega_L + i \tan(L\Omega_L)(E\gamma(0) + \Delta_L)}{\Omega_L - i \tan(L\Omega_L)(E - \gamma(0)\tilde{\Delta}_L)} \\ \gamma(2L) &= \frac{\gamma(L)\Omega_{2L} + i \tan(L\Omega_{2L})(E\gamma(L) + \Delta_{2L})}{\Omega_{2L} - i \tan(L\Omega_{2L})(E - \gamma(L)\tilde{\Delta}_{2L})}, \end{aligned}$$

Due to the periodicity of solution it is demanded that  $\gamma(2L) = \gamma(0)$ . Also in the considered problem I presume the existence of rotational symmetry in xy-plane. This allows me to consider trajectories with  $p_y$  component equal to zero as solution with non-zero  $p_y$  can always be obtained by rotation of the coordinate system.

## 4.1 No collision trajectory solution.

In this limit trajectory is parallel to one of the boundaries, meaning that the quasiparticle never experience reflection with other boundary and travels in the same homogeneous potential as it shown on Fig.4.2. In that case any initial condition value will eventually converge towards a homogeneous solution corresponding to the value of the order parameter near the boundary.



**Figure 4.2:** Scheme of the considered case. The green dots represent initial and final points. Both of them are infinitely distant.

Keeping that in mind lets consider a part of trajectory where solution starts with initial value  $\gamma(0)$  travel along the trajectory for arbitrary distance  $L$  obtaining the same value  $\gamma(0)$

as it started from. Plugging it in formula (4.3) we obtain:

$$\gamma(0) = \frac{\gamma(0)\Omega_L + i \tan(L\Omega_L)(E\gamma(0) + \Delta_L)}{\Omega_L - i \tan(L\Omega_L)(E - \gamma(0)\tilde{\Delta}_L)}.$$

Or after some simplification one will obtain:

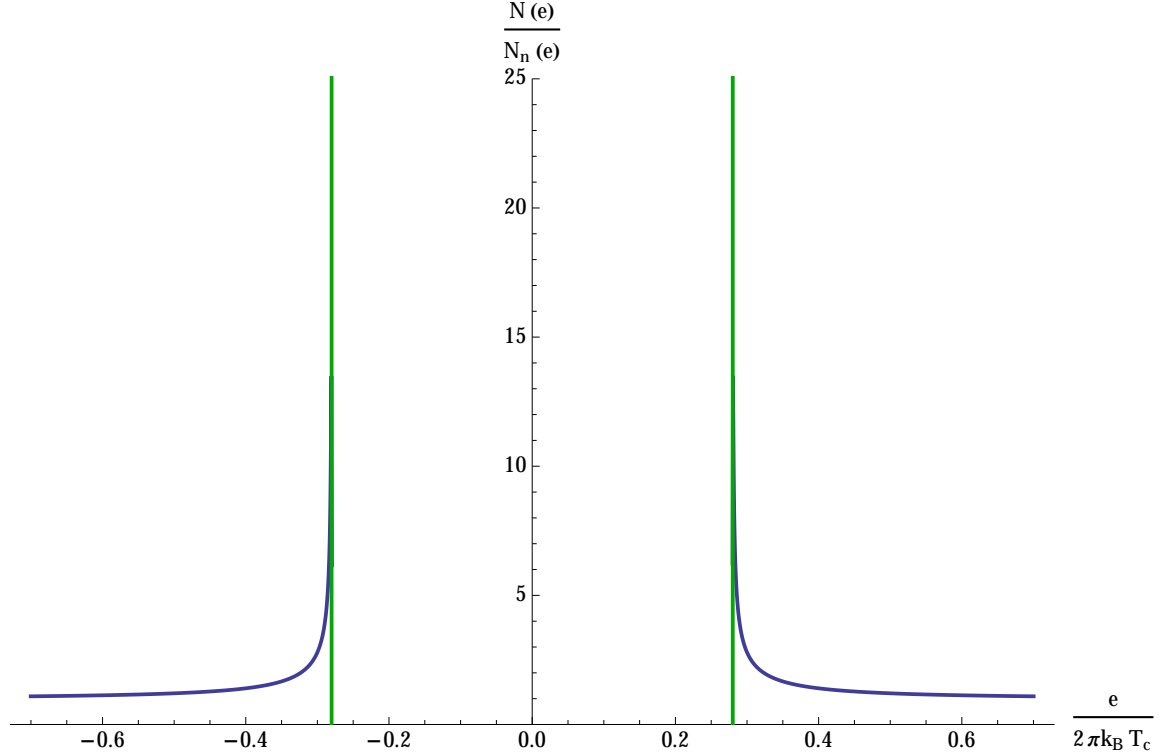
$$-\gamma(0)\tilde{\Delta}_L\gamma(0) + 2E\gamma(0) + \Delta_L = 0 \quad (4.4)$$

This equation is a matrix Ricatti equation for the homogeneous case of the order parameter. So as we correctly guessed before  $\gamma(0) = \gamma_h$ . There is a way to obtain solution to homogeneous Ricatti equation using only linear algebra which I presented before and it goes as follows:

$$\gamma_h = \tilde{\Delta}_L^{-1} \left( E - \sqrt{E^2 - \Delta^2} \right) = \frac{E - \sqrt{E^2 - \Delta^2}}{\Delta} \sigma_z,$$

where  $\Delta_L = -\tilde{\Delta}_L = \Delta\sigma_x \cdot i\sigma_y$  for the case of trajectory with no impact. Solution for  $\tilde{\gamma}_h$  can be obtained similarly or by using "tilde" symmetry relation as it defined in the end of sub chapter 2.5 to (4.4). This allows to obtain well-known picture of a bulk density of states for a superconductor:





**Figure 4.3:** Bulk density of states that is realised for trajectory with no collisions. Green lines - value of  $\pm\Delta_B$ .

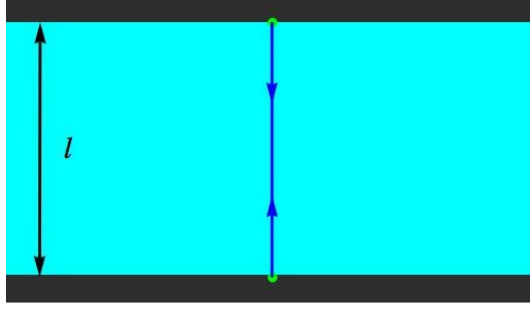
## 4.2 Normal impact trajectory solution.

Normal impact trajectory is the second important limit to consider in the given problem. In this limit quasiparticle experiences most of collisions per unit length travelled, meaning that boundary effects should be represented at their strongest. Trajectory for that case is presented on Fig.4.4. Once again, I will use the formula (4.3) for quasiparticle to travel until first collision (index  $L$ ) and return back after it (index  $2L$ ):

$$\gamma(L) = \frac{\gamma(0)\Omega_L + i \tan(l\Omega_L)(E\gamma(0) + \Delta_L)}{\Omega_L - i \tan(l\Omega_L)(E - \gamma(0)\tilde{\Delta}_L)}$$

$$\gamma(0) = \frac{\gamma(L)\Omega_{2L} + i \tan(l\Omega_{2L})(E\gamma(L) + \Delta_{2L})}{\Omega_{2L} - i \tan(l\Omega_{2L})(E - \gamma(L)\tilde{\Delta}_{2L})},$$

here  $\Delta_L = -\Delta_{2L}$ . Because of that  $\Omega_L = \Omega_{2L} = -\sqrt{E^2 - \Delta\tilde{\Delta}}$  and will be called  $\Omega$ . In this formulas  $L$  is the distance between collisions and is equal to the distance between boundaries



**Figure 4.4:** Scheme of the normal collision case. The green dots represent reflection points. Periodic boundary condition is assumed for that trajectory.

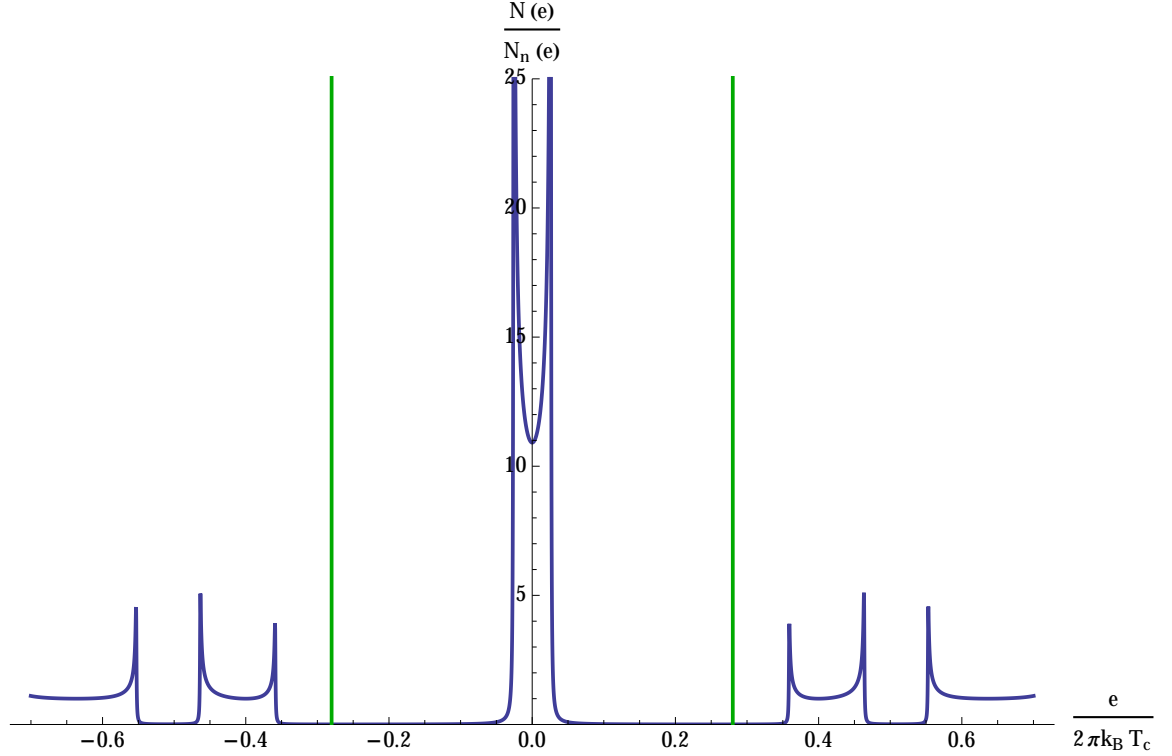
for normal impact. Taking into account that  $\Delta_L = -\tilde{\Delta}_L = \Delta\sigma_z \cdot i\sigma_y$  one will obtain equation:

$$-\gamma\tilde{\Delta}_L\gamma + 2\frac{i\Omega}{\tan(l\Omega)}\gamma - \Delta_L = 0.$$

As one could see this equation have the same form as homogeneous equation with a different coefficient corresponding to energy. In that case one can obtain solution for that equation in a similar manner:

$$\gamma_{\perp} = \tilde{\Delta}_L^{-1} \left( \frac{i\Omega}{\tan(l\Omega)} - \sqrt{\left( \frac{i\Omega}{\tan(l\Omega)} \right)^2 + \Delta^2} \right) = \frac{i \left( \Omega - \sqrt{\Omega^2 - \Delta^2 \tan^2(l\Omega)} \right)}{\Delta \tan(l\Omega)} \sigma_x$$

With gamma obtained one can get a local density of states at the boundary for normal impact trajectory:



**Figure 4.5:** Desntiy of states for trajectory perpendicular to the boundaries. Green lines - value of  $\pm\Delta$ .

### 4.3 General equation for one collision problem

In two previous examples when deriving the solutions we came across some sort of matrix Ricatti equation. This brings one to thought of deriving a general equation for one collision problem where quasiparticle scatters specularly from region with order parameter  $\Delta_L$  to region with order parameter  $\Delta_{2L}$ .

Specular reflection makes  $\Delta_L$  differ from  $\Delta_{2L}$  by sign of component dependent of  $p_z$ . In order to use the formula (4.3) one has to ensure that  $E$  and  $\Omega$  are diagonal matrices. In our case it is provided by disregard of self-energies  $\Sigma$  and considering pure triplet order parameter  $\Delta$  so that  $\Delta^2 \propto \sigma_0$ . Given that the order parameter before the collision differs from one after it only by sign of component proportional to  $p_z$  it is easy to check that  $\Delta_L^2 = \Delta_{2L}^2$ . As a consequence of this  $\Omega_L = \Omega_{2L} \equiv \Omega$  which would further simplify our calculation. Starting with

formulas giving solution before and after impact and using periodicity condition  $\gamma(2L) = \gamma(0)$ :

$$\begin{aligned}\gamma(L) &= \frac{(\Omega + iE \tan(L\Omega))\gamma(0) + i \tan(L\Omega)\Delta_L}{(\Omega - iE \tan(L\Omega)) + i \tan(L\Omega)\gamma(0)\tilde{\Delta}_L}, \\ \gamma(0) &= \frac{(\Omega + iE \tan(L\Omega))\gamma(L) + i \tan(L\Omega)\Delta_{2L}}{(\Omega - iE \tan(L\Omega)) + i \tan(L\Omega)\gamma(L)\tilde{\Delta}_{2L}}.\end{aligned}$$

If we presume that the denominator of the first expression is an invertible matrix and would abbreviate repeating expressions, we would end up with the following equation:

$$\begin{aligned}((\Omega - iETn)^2 + iTn(\Omega - iETn)\gamma(0)\tilde{\Delta}_L + iTn(\Omega + iETn)\gamma(0)\tilde{\Delta}_{2L} - ETn^2\Delta_L\tilde{\Delta}_{2L})\gamma(0) = \\ ((\Omega + iETn)^2 + i \tan(\Omega + iETn)\Delta_L + i \tan(\Omega - iETn)\Delta_{2L} - ETn^2\gamma(0)\tilde{\Delta}_L\Delta_{2L}),\end{aligned}$$

where  $\tan(L\Omega)$  was substituted for  $Tn$  to make expression look less bulky. After expanding brackets and grouping up elements following equation is obtained:

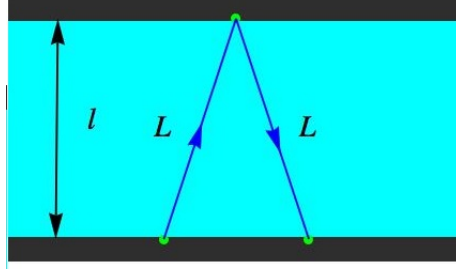
$$\begin{aligned}\gamma(\Omega(\tilde{\Delta}_{2L} + \tilde{\Delta}_L) + iE \tan(L\Omega)(\tilde{\Delta}_{2L} - \tilde{\Delta}_L))\gamma + i \tan(L\Omega)(\Delta_L\tilde{\Delta}_{2L}\gamma - \gamma\tilde{\Delta}_L\Delta_{2L}) - \\ - 4E\Omega\gamma - \Omega(\Delta_{2L} + \Delta_L) - iE \tan(L\Omega)(\Delta_L - \Delta_{2L}) = 0\end{aligned}\tag{4.5}$$

This equation gives solution for periodic coherence amplitudes that are scattered from a region with order parameter  $\Delta_L$  to the region with order parameter  $\Delta_{2L}$ . In that expression  $L$  is a distance between consequent collisions along chosen trajectory.

#### 4.4 Non-normal collision trajectory solution.

Now solution can be obtained for the case of any direction of quasiparticle trajectory as shown on Fig.4.6. The problem has a rotational symmetry along z-axis one can put  $p_y = 0$  and consider  $\Delta_L = \Delta(p_x * \sigma_x + p_z * \sigma_z) \cdot i\sigma_y$  as the order parameter in the problem, where  $p_i$  are components of the unit vector in momentum space. Given that, one can calculate coefficients in (4.5) and obtain the following:

$$\begin{aligned}\gamma(\Omega(\Omega \sin(\theta)\sigma_z - iE \tan(L\Omega) \cos(\theta)\sigma_x)\gamma - \frac{\Delta}{2} \tan(L\Omega) \sin(2\theta)(\sigma_y\gamma - \gamma\sigma_y) - \\ - \frac{2E\Omega}{\Delta}\gamma + \Omega \sin(\theta)\sigma_z + iE \tan(L\Omega) \cos(\theta)\sigma_x = 0,\end{aligned}$$



**Figure 4.6:** Scheme for the non-normal collision case. The green dots represent reflection points. Periodic boundary condition is assumed for that trajectory.

where  $L = \frac{l}{\cos(\theta)}$  is the distance between collisions along the trajectory and  $l$  is the distance between boundaries. The obtained equation looks like sum of two equations considered before with the addition of a term  $\frac{\Delta}{2} \tan(L\Omega) \sin(2\theta)(\sigma_y \gamma - \gamma \sigma_y)$ , giving me a reason to look for the solution in the form of linear combination of Pauli matrices from both of the solutions:

$$\gamma = a * \sigma_x + b * \sigma_z.$$

After substituting this ansatz into obtained previously equation, one would get following system of equations:

$$\begin{cases} iE \tan(L\Omega) \cos(\theta)(b^2 - a^2) + 2\Omega \sin(\theta) * ab - \frac{2E\Omega}{\Delta} a + iE \tan(L\Omega) \cos(\theta) - i\Delta \tan(L\Omega) \sin(2\theta)b = 0, \\ \Omega \sin(\theta)(b^2 - a^2) - 2iE \tan(L\Omega) \cos(\theta) * ab - \frac{2E\Omega}{\Delta} b + \Omega \sin(\theta) + i\Delta \tan(L\Omega) \sin(2\theta)a = 0. \end{cases} \quad (4.6)$$

This system can be transformed into a system of two independent equations if variable substitution of this sort is considered:

$$\begin{aligned} t &= \frac{a + ib}{2}, \\ z &= \frac{a - ib}{2}. \end{aligned}$$

In system with new variables I consider two linear combinations of equations from the previous system to obtain the following system of two independent quadratic equations:

$$\begin{cases} 4 * (\Omega \sin(\theta) + E \tan(L\Omega) \cos(\theta))t^2 - 2i(\frac{2E\Omega}{\Delta} + \Delta \tan(L\Omega) \sin(2\theta))t - \\ - (\Omega \sin(\theta) + E \tan(L\Omega) \cos(\theta)) = 0, \\ 4 * (\Omega \sin(\theta) - E \tan(L\Omega) \cos(\theta))z^2 - 2i(\Delta \tan(L\Omega) \sin(2\theta) - \frac{2E\Omega}{\Delta})z - \\ - (\Omega \sin(\theta) - E \tan(L\Omega) \cos(\theta)) = 0. \end{cases}$$

Both of the equations have two solutions and in order to write them down I will introduce two following functions:

$$\begin{aligned} T &= \frac{\frac{2E\Omega}{\Delta} + \Delta \tan(\frac{l}{\cos(\theta)}\Omega) \sin(2\theta)}{\Omega \sin(\theta) + E \tan(\frac{l}{\cos(\theta)}\Omega) \cos(\theta)}, \\ Z &= \frac{\Delta \tan(\frac{l}{\cos(\theta)}\Omega) \sin(2\theta) - \frac{2E\Omega}{\Delta}}{\Omega \sin(\theta) - E \tan(\frac{l}{\cos(\theta)}\Omega) \cos(\theta)}. \end{aligned}$$

In terms of these functions solution for the equation on  $\gamma$  will take form:

$$\gamma = \frac{i}{4}(T + Z \pm \sqrt{T^2 - 4} \pm \sqrt{Z^2 - 4})\sigma_x + \frac{1}{4}(T - Z \pm \sqrt{T^2 - 4} \mp \sqrt{Z^2 - 4})\sigma_z \quad (4.7)$$

In order to obtain full information about the system one needs to solve independent equation for  $\tilde{\gamma}$  that is obtained by performing  $\sim$  operation over the equation (4.5). The analytical solution to that equation is obtained via repeating the procedure described previously. Which results in the following expression:

$$\tilde{\gamma} = -\frac{i}{4}(T + Z \pm \sqrt{T^2 - 4} \pm \sqrt{Z^2 - 4})\sigma_x + \frac{1}{4}(T - Z \pm \sqrt{T^2 - 4} \mp \sqrt{Z^2 - 4})\sigma_z \quad (4.8)$$

Choice of sign in front of the square roots determined by the fact that one should obtain a "physical solution". By "physical solution" I mean solution with positive density of states and spectral densities of states. Such solution should also be stable along the trajectory which allows to develop a criterion.

Let's start from linearising Ricatti equation with respect to homogeneous solution:

$$i\partial\gamma = \gamma(\tilde{E} + 0.5 * \tilde{\Delta}\gamma) - (E - 0.5\gamma\tilde{\Delta})\gamma - \Delta,$$

$$i\partial(\gamma_h + \delta\gamma) = (\gamma_h + \delta\gamma)(\tilde{E} + 0.5 * \tilde{\Delta}(\gamma_h + \delta\gamma)) - (E - 0.5(\gamma_h + \delta\gamma)\tilde{\Delta})(\gamma_h + \delta\gamma) - \Delta,$$

$$i\partial\delta\gamma \approx \delta\gamma(\tilde{E} + \tilde{\Delta}\gamma_h) - (E - \gamma_h\tilde{\Delta})\delta\gamma$$

now for  $\delta\gamma = 0$  solution of obtained equation to be stable we need to demand that all real parts of eigenvalues of both matrices should have negative real part which will result in inequalities:

$$\text{Im}\Lambda[(\tilde{E} + \tilde{\Delta}\gamma_h)] > 0, \quad (4.9a)$$

$$\text{Im}\Lambda[(E - \gamma_h\tilde{\Delta})] < 0. \quad (4.9b)$$

Where  $\text{Im}\Lambda[\dots]$  stands for imaginary part of every eigenvalue of the considered matrix. Concluding same manipulations for equation on "tilded" gammas one would get:

$$\text{Im}\Lambda[(\tilde{E} + \tilde{\Delta}\tilde{\gamma}_h)] > 0, \quad (4.10a)$$

$$\text{Im}\Lambda[(\tilde{E} - \tilde{\gamma}_h\tilde{\Delta})] < 0. \quad (4.10b)$$

these restrictions should be fulfilled in every point of the trajectory.

## 4.5 Density of states for 3He-B in 1D confinement.

As seen from before analytical solution for the problem considered expression for DoS seems to be rather bulky and hard to grasp intuitively. In order to simplify obtained relation and get insight into the system's density of states I will do a Taylor expansion of solution over impact angle  $\theta$  assuming it being small. Obviously, as DoS should be even function of incident angle, one needs to expand it at least to 2nd term in order to capture essential function behaviour at small angles.

Lets start with expanding  $\tan(\frac{l}{\cos(\theta)}\Omega)$  term that can be found in both coefficients forming

solution, remembering some trigonometric identities one will get the following:

$$\begin{aligned}\tan\left(\frac{l\Omega}{\cos(\theta)}\right) &\approx \tan\left(\frac{l\Omega}{1 - 0.5 * \theta^2}\right) \approx \tan\left(l\Omega(1 + \frac{\theta^2}{2})\right) = \frac{\tan(l\Omega) + \tan(\frac{l\Omega}{2}\theta^2)}{1 - \tan(l\Omega)\tan(\frac{l\Omega}{2}\theta^2)} \approx \\ &\approx \left(\tan(l\Omega) + \frac{l\Omega}{2}\theta^2\right) \left(1 + \tan(l\Omega)\frac{l\Omega}{2}\theta^2\right) \approx \tan(l\Omega) + (1 + \tan^2(l\Omega))\frac{l\Omega}{2}\theta^2 = \\ &= \tan(l\Omega) + \frac{l\Omega}{2\cos^2(l\Omega)}\theta^2\end{aligned}$$

With that step done  $T$  and  $Z$  functions can be expanded in powers of  $\theta$  in order to proceed with the expansion:

$$\begin{aligned}T &\approx \frac{\frac{2\Omega E}{\Delta} + 2\Delta(\tan(l\Omega) + \frac{l\Omega}{2\cos^2(l\Omega)}\theta^2)\theta}{E(\tan(l\Omega) + \frac{l\Omega}{2\cos^2(l\Omega)}\theta^2) + \Omega\theta} \approx \frac{\frac{2\Omega E}{\Delta} + 2\Delta \tan(l\Omega)\theta}{E \tan(l\Omega) + \Omega\theta + \frac{El\Omega}{2\cos^2(l\Omega)}\theta^2} \approx \\ &\approx \frac{2}{E \tan(l\Omega)} \left(\frac{\Omega E}{\Delta} + \Delta \tan(l\Omega)\theta\right) \left(1 - \frac{\Omega}{E \tan(l\Omega)}\theta + \left(\frac{\Omega^2}{E^2 \tan^2(l\Omega)} - \frac{l\Omega}{\sin(2l\Omega)}\right)\theta^2\right) \approx \\ &\approx \frac{2\Omega}{\Delta \tan(l\Omega)} + 2\left(\frac{\Delta}{E} - \frac{\Omega^2}{\Delta E \tan^2(l\Omega)}\right)\theta + \frac{2\Omega}{\Delta \tan(l\Omega)} \left(\frac{\Omega^2}{E^2 \tan^2(l\Omega)} - \frac{l\Omega}{\sin(2l\Omega)} - \frac{\Delta^2}{E^2}\right)\theta^2 \equiv \\ &\equiv \frac{2\kappa}{\Delta} + 2\left(\frac{\Delta}{E} - \frac{\kappa^2}{\Delta E}\right)\theta + \frac{2\kappa}{\Delta} \left(\frac{\kappa^2}{E^2} - \frac{l\Omega}{\sin(2l\Omega)} - \frac{\Delta^2}{E^2}\right)\theta^2,\end{aligned}$$

similarly:

$$Z \approx \frac{\frac{2\Omega E}{\Delta} - 2\Delta(\tan(l\Omega) + \frac{l\Omega}{2\cos^2(l\Omega)}\theta^2)\theta}{E(\tan(l\Omega) + \frac{l\Omega}{2\cos^2(l\Omega)}\theta^2) - \Omega\theta} \approx \frac{2\kappa}{\Delta} + 2\left(\frac{\kappa^2}{\Delta E} - \frac{\Delta}{E}\right)\theta + \frac{2\kappa}{\Delta} \left(\frac{\kappa^2}{E^2} - \frac{l\Omega}{\sin(2l\Omega)} - \frac{\Delta^2}{E^2}\right)\theta^2.$$

One could expand  $\sqrt{T^2 - 4}$  and  $\sqrt{Z^2 - 4}$  to obtain following expressions:

$$\begin{aligned}T + Z &= \frac{4\kappa}{\Delta} + \frac{4\kappa}{\Delta} \left(\frac{\kappa^2}{E^2} - \frac{l\Omega}{\sin(2l\Omega)} - \frac{\Delta^2}{E^2}\right)\theta^2, \\ T - Z &= 4\left(\frac{\Delta}{E} - \frac{\kappa^2}{\Delta E}\right)\theta, \\ \sqrt{T^2 - 4} + \sqrt{Z^2 - 4} &= 4\sqrt{\kappa^2 - 1} + \frac{2}{\sqrt{\kappa^2 - 1}} \left(\left(\frac{\Delta}{E} - \frac{\kappa^2}{\Delta E}\right)^2 + \frac{2\kappa^2}{\Delta^2} \left(\frac{\kappa^2}{E^2} - \frac{l\Omega}{\sin(2l\Omega)} - \frac{\Delta^2}{E^2}\right) - \frac{\kappa}{\Delta^2 \tan(l\Omega)(\kappa^2 - 1)} \left(\frac{\Delta}{E} - \frac{\kappa^2}{\Delta E}\right)^2\right)\theta^2, \\ \sqrt{T^2 - 4} - \sqrt{Z^2 - 4} &= \frac{4\kappa}{\Delta\sqrt{\kappa^2 - 1}} \left(\frac{\Delta}{E} - \frac{\kappa^2}{\Delta E}\right)\theta.\end{aligned}$$



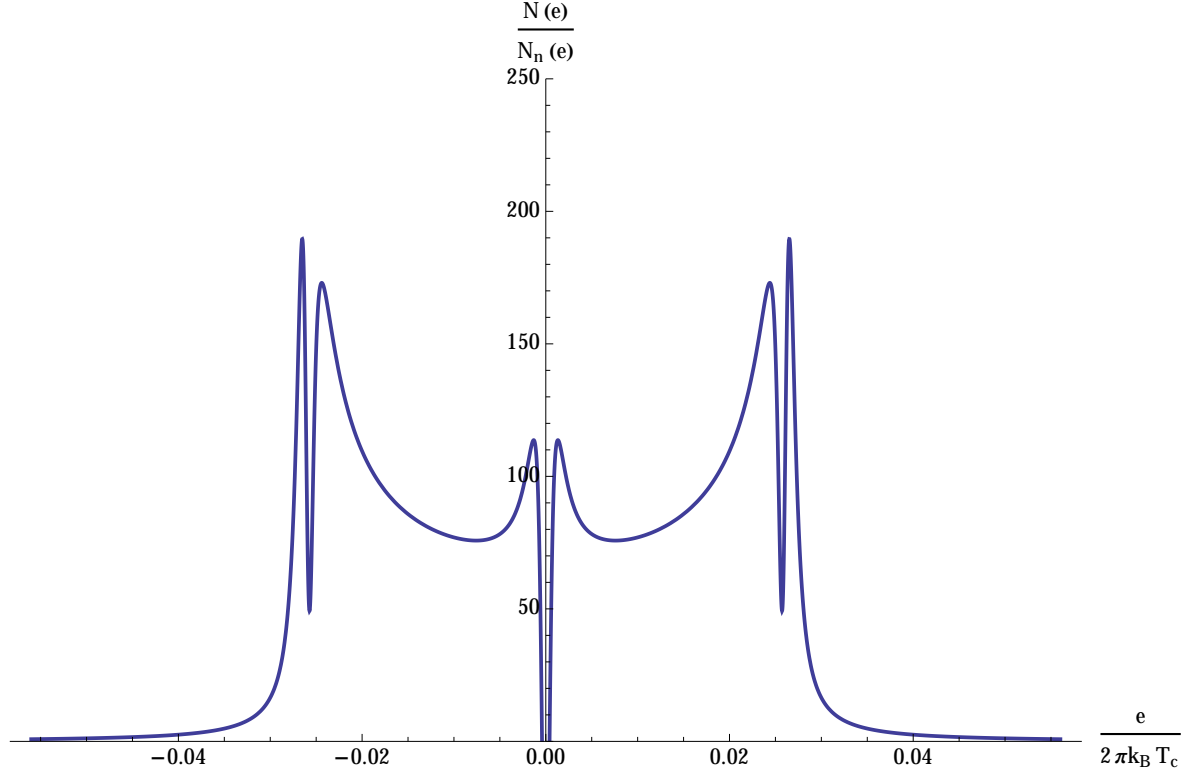
This gives a dependence of solution for  $\gamma$  and  $\tilde{\gamma}$  from  $\theta$  up to second order:

$$\begin{aligned}\gamma &= \frac{i}{4}(C_1 + C_2\theta^2)\sigma_x + \frac{1}{4}(C_3\theta)\sigma_z, \\ \tilde{\gamma} &= -\frac{i}{4}(C_1 + C_2\theta^2)\sigma_x + \frac{1}{4}(C_3\theta)\sigma_z.\end{aligned}$$

Then the density of states up to second order in  $\theta$  would stand as follows:

$$\begin{aligned}\frac{N(\epsilon, \theta)}{N_F} &= -\frac{1}{2\pi} \text{Im} \left( \text{Tr} \left( -i\pi \frac{1 + \gamma\tilde{\gamma}}{1 - \gamma\tilde{\gamma}} \right) \right) \approx \frac{1}{2} \text{Re} \left( \text{Tr} \left( \frac{(1 + \frac{C_1^2}{16} + \frac{2C_1C_2 + C_3^2}{16}\theta^2)\sigma_0 + \frac{C_1C_3}{8}\theta\sigma_y}{(1 - \frac{C_1^2}{16} - \frac{2C_1C_2 + C_3^2}{16}\theta^2)\sigma_0 - \frac{C_1C_3}{8}\theta\sigma_y} \right) \right) = \\ &= \text{Re} \left( \frac{1 - \left( \frac{C_1^2 + (2C_1C_2 + C_3^2)\theta^2}{16} \right)^2 + \frac{C_1^2C_3^2}{64}\theta^2}{\left( 1 - \frac{C_1^2 + (2C_1C_2 + C_3^2)\theta^2}{16} \right)^2 - \frac{C_1^2C_3^2}{64}\theta^2} \right) \approx \frac{1 - \frac{C_1^4}{16^2} - \frac{C_1^2(C_1C_2 - C_3^2)}{128}\theta^2}{\left( 1 - \frac{C_1^2}{16} \right)^2 - \left( \frac{(1 - \frac{C_1^2}{16})(2C_1C_2 + C_3^2)}{8} + \frac{C_1^2C_3^2}{64} \right)\theta^2} \approx \\ &\approx \frac{1 + \frac{C_1^2}{16}}{1 - \frac{C_1^2}{16}} - \left( \frac{4 \left( 1 - \frac{C_1^2}{16} \right) (2C_1C_2 + C_3^2) + C_1^2C_3^2}{32 \left( 1 - \frac{C_1^2}{16} \right)^3} \right) \theta^2\end{aligned}$$

One can check that zero order term with  $C_1 = 4 \left( \frac{\kappa}{\Delta} - \sqrt{\kappa^2 - 1} \right)$  is identical to the density of states obtained for normal trajectory while the second order term will be responsible for splitting zero energy band in two for small incident angles as shown on the figure:



**Figure 4.7:** The density of states on the boundary of a slab for slightly non-normal collision trajectory.

## 4.6 Problem outlook.

This problem has been considered with two intentions. First, is to have a problem with a solution that can be obtained analytically and compare it with the program output in order to validate the code. Second, is to get some insight in  $^3\text{He}$  physics in the confinement only by an analytical approach. This approach has a disadvantage of producing bands at energies higher than superconducting gap which contradicts with the previous paper [52], but on the other hand, reproduces exact position of the bound states inside the gap. The previous section proves a point that zero energy states exist only for the normal impact trajectory and even the slightest declination from the normal impact would destroy zero energy bound state. Henceforth only spectral LDOS of a normal impact trajectory 2.31 plays a role in the zero energy states discussion, while all the other trajectories do not describe that state. The contradiction that arises in analytical solution with the previous results is only due to the initial assumption that the superconducting gap is not affected by the boundaries. In other

words, it allows for multiple reflections from the boundaries to have a zero net phase along the trajectory thus creating Andreev bound states for energies above the gap.

## Chapter 5

# Magnetic scattering boundaries in 1D confinement.

### 5.1 Motivation.

The problem of  $^3\text{He}$  confined in one dimension is well studied both numerically and experimentally [1, 16, 17, 20, 25]. Experimentally it is hard to produce an atomically smooth surface. On the other hand, it was shown by the theory that superfluidity in  $^3\text{He}$  is heavily suppressed by rough surfaces. In order to overcome this issue in experiment researchers add some quantities of  $^3\text{He}$  or  $^4\text{He}$  to be deposited on the surface, smoothening it as schematically shown in Fig. 5.1. It is known that this sort of "coating" has ferromagnetic properties which allow considering a problem where the boundaries of the container have magnetic properties. Depending on a size of a slab  $d$  superfluid order parameter takes different forms corresponding to different phases of the superfluid  $^3\text{He}$ . Here I take an attempt into exploring and explaining how magnetic scattering on the boundaries affect  $^3\text{He}$  superfluidity and how it is different to a known case of  $^3\text{He}$  in a slab [52].



**Figure 5.1:** Schematic representation of a slab with a coating.

## 5.2 Numerical approach and tips.

The calculation is split into two parts. First, after defining boundary conditions, I solve Eilenberger equation (2.29) for retarded Green's function in Matsubara frequencies. The second step, I solve Eilenberger equation in real energies using obtained order parameter spatial dependence as an input. This allows calculating the density of states of the system without using somehow a notorious analytical continuation of Matsubara Green's function. Matsubara Green's function is obtained by treating time as an imaginary temperature [53]. Matsubara Green's function has periodic poles along the imaginary axis that are called Matsubara frequencies, for fermions these frequencies obey the equation  $iE_n = i\pi T(2n + 1)$ , where  $n \in \mathbb{Z}$ . With substitution  $E \rightarrow iE_n$  the Eilenberger equation would read:

$$[iE_n - \underline{\sigma}^M, \underline{g}^M]_{\odot} + i\hbar v_F \nabla_{\mathbf{R}} \underline{g}^M = 0, \quad (5.1)$$

with the difference that now all integrals over energies are substituted by summation over the poles of Matsubara's Green's function. Gap equation (2.34) for triplet pairing in Matsubara notation will take form:

$$\Delta(\mathbf{p}, \mathbf{R}, t) = k_B T \sum_{|E_n| < E_c} \int \frac{d\Omega_{\mathbf{p}'}}{4\pi} 3V_t(\mathbf{p} \cdot \mathbf{p}') f^M(\mathbf{p}', \mathbf{R}, E_n, t), \quad (5.2)$$

This equation can be simplified following procedure presented in [54]. Performing it will hold:

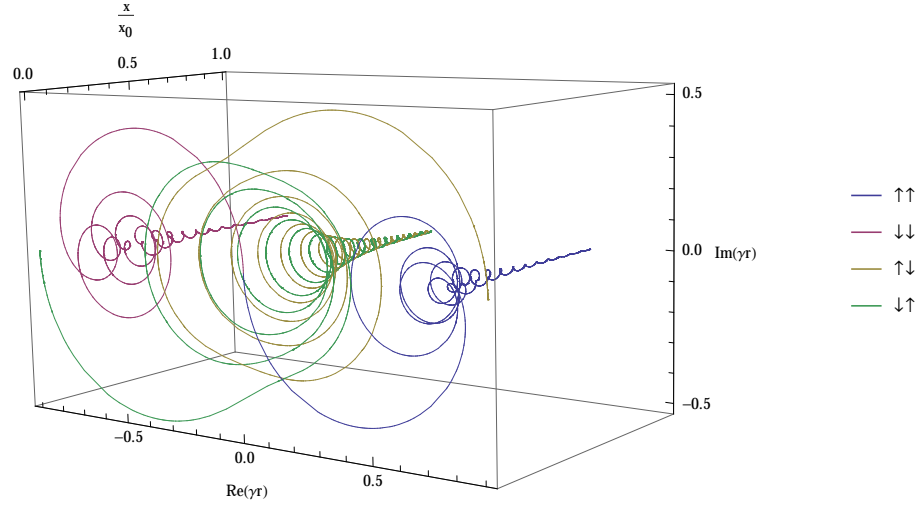
$$\Delta(\mathbf{p}, \mathbf{R}, t) \ln \left( \frac{T}{T_C} \right) = k_B T \sum_{|E_n|} \left( \int \frac{d\Omega_{\mathbf{p}'}}{4\pi} (\mathbf{p} \cdot \mathbf{p}') f_{i,j}^M(\mathbf{p}', \mathbf{R}, E_n, t) - \pi \frac{\Delta(\mathbf{p}, \mathbf{R}, t)}{|E_n|} \right).$$

This procedure allows to eliminate the cut-off and elude divergence at high energies in the sum by subtracting high energy behaviour of  $f^M$ .

When talking about numerical procedure, there is another mistake that could be easily done by a researcher. When one calculates the average of a function over the Fermi surface there is a goal of performing average precisely at least up to the leading order of integrated function. In case of averaging  $\mathbf{p}' f_{i,j}^M(\mathbf{p}', \mathbf{R}, E_n, t) \equiv \mathbf{p}'^2$ , meaning that best integration procedure to obtain an exact answer is a well known Simpson rule. Second hindrance that can result in underestimating some of the order parameter values in iteration procedure comes from term  $d\Omega_{\mathbf{p}'}$ , which in terms of spherical coordinates turns into  $\sin(\theta)d\theta d\phi$ . An under or an overestimation of the order parameter components due to miscalculation of integral of  $\sin(\theta)$  can be solved by increasing amount of trajectories varying  $p_z$  component, but in order to reach desired precision one would need to take around 1000 different uniformly distributed directions which is a considerable step down in performance in the case of my program. Another way is also well known substitution of variables instead of taking integral over  $\sin(\theta)d\theta$  and considering  $f(\theta)$  one could consider  $-d(\cos(\theta))$  and  $f(\cos(\theta))$ . This substitution allows to reach desired precision without increasing the number of trajectories. The first step computationally advantageous as it allows not to solve equations for functions parametrising Keldysh component of Green's function. Another advantage is that Matsubara frequencies are purely imaginary, allowing to obtain right initial conditions faster. Another important feature for both steps is to explain how numerical procedure is carried on. Equation on coherence amplitudes for both Matsubara and retarded component of Keldysh contour Green's function is having the same form. Meaning, that procedure described further will hold for both cases.

The first step would be to break down our calculation area into small regions in which we assume that order parameter is constant. Important is that in further calculations, we should take an order parameter value in the middle of this region in order to ensure that forward and backward trajectory travels through the identical order parameter profile.

For each region where we consider the order parameter value to be constant we can simplify



**Figure 5.2:** Convergence along the trajectory of some initial conditions in case of homogeneous order parameter. Magnitude of the imaginary part of the energy corresponds to decay rate of illustrated oscillations.

the equation presented in chapter with Ricatti parametrisation (2.39). For homogeneous case this formula reduces to (4.2), allowing to express solution dependence along the trajectory via matrix exponents.

The last step would be to determine appropriate initial conditions. In my problem I consider only solutions that are periodic after two reflections from the boundaries. Last but not least, knowing  $\gamma^R, \tilde{\gamma}^R$  I am able to obtain spectral function via following formula:

$$\frac{N(\mathbf{p}, E)}{N_F} = -\frac{1}{\pi} \text{Im}\{\text{Tr} [\mathcal{G}^R(\mathbf{p}, E)]\}. \quad (5.3)$$

### 5.3 BW and planar phase solutions.

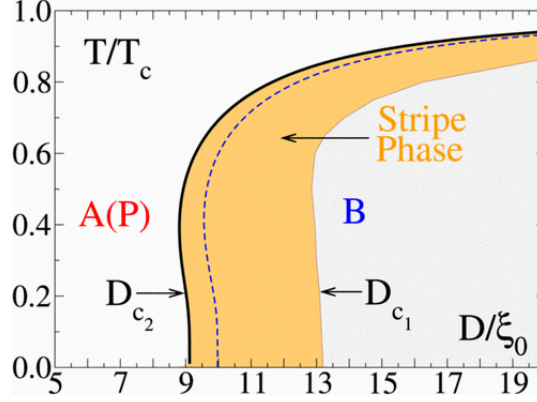
In order to obtain a zero-energy states a following form of the order parameter is considered [20–22]:

$$\begin{pmatrix} \Delta_{\parallel}(z) & 0 & 0 \\ 0 & \Delta_{\parallel}(z) & 0 \\ 0 & 0 & \Delta_{\perp}(z) \end{pmatrix}.$$

This form of order parameter corresponds to a  $^3\text{He}$  confined in a slab.

It resembles the order parameter form of a bulk B phase, but with distorted component that corresponds to pairs with their momentum perpendicular to slab boundaries.

Behaviour of order parameter was studied in the article [1], in which a dependence of the superfluid phase from the distance between the boundaries in the slab was established. As I



**Figure 5.3:** T-D phase diagram of  $^3\text{He}$  considered in weak-coupling limit ( $P=0$ ). Obtained by [1].

consider one dimensional problem a stripe phase solution is out of the scope of my calculations. Consequently, for me the meaning of their research reduces to: if the slab is thicker than  $10\xi_0$  B-phase is stable, while if lower  $\Delta_\perp(z)$  becomes suppressed and order parameter starts to describe planar phase:

$$\begin{pmatrix} \Delta_{pl} & 0 & 0 \\ 0 & \Delta_{pl} & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

which, as we know from the previous chapter, is unstable and then becomes another known stable phase – A phase. To confirm that my calculations are in line with these results I obtained solutions presented on figure 5.4.

My calculations show that boundaries with magnetic scattering change the phase diagram discussed before. In order to confirm the results of numerical calculations let us consider a simple analytical problem: a magnetic boundary with specular scattering in quasi-classical approach. In that problem I would neglect usual suppression of order parameter near boundaries, allowing to consider  $\gamma$  as a homogeneous solution:

$$\gamma(p) = -\frac{\hat{\Delta}(\mathbf{p})}{E + i\sqrt{|\Delta|^2 - E^2}}i\sigma_y, \quad \tilde{\gamma}(\underline{p}) = i\sigma_y \frac{\hat{\Delta}^*(\mathbf{p})}{E + i\sqrt{|\Delta|^2 - E^2}}i\sigma_y.$$

Also, I would assume that spin space and orbital space axes coincide, allowing to consider





the last term in that expression represents singlet correlations appearing due to a magnetic scattering on the boundaries. Which brings me back to the determinant:

$$\begin{aligned} \det \left[ \hat{1} - \left( E + i\sqrt{|\Delta|^2 - E^2} \right)^{-2} \left( \hat{\Delta}(\mathbf{p}) - 2\sin^2(0.5\nu)\Delta(\mathbf{m}\mathbf{p})(\mathbf{m}\boldsymbol{\sigma}) + i\sin(\nu)\Delta(\mathbf{m}\mathbf{p})\hat{1} \right) \hat{\Delta}^*(\mathbf{p}) \right] = \\ = \left[ \hat{1} - \left( E + i\sqrt{|\Delta|^2 - E^2} \right)^{-2} \left( \Delta^2(\mathbf{p}\mathbf{p})\hat{1} + \Delta^2(\mathbf{p} \times \mathbf{p})\boldsymbol{\sigma} - 2\sin^2(0.5\nu)\Delta^2(\mathbf{m}\mathbf{p})((\mathbf{m}\mathbf{p})\hat{1} + \right. \right. \\ \left. \left. + (\mathbf{m} \times \mathbf{p})\boldsymbol{\sigma}) + i\sin(\nu)\Delta(\mathbf{m}\mathbf{p})\hat{\Delta}^*(\mathbf{p}) \right) \right] = 0 \end{aligned}$$

Following an identity  $\det [p_0\hat{1} + (\mathbf{p}\boldsymbol{\sigma})] = p_0^2 - p_x^2 - p_y^2 - p_z^2$  determinant expression would be reduced to:

$$\frac{E}{\Delta} \pm \sqrt{\frac{(\mathbf{p}\mathbf{p}) + 1}{2} - (\mathbf{m}\mathbf{p})(\mathbf{m}\mathbf{p})\sin^2(0.5\nu)} = 0$$

Dividing momenta into components perpendicular and parallel to a surface expression reduces to:

$$\frac{E}{\Delta} = \pm \sqrt{p_{\parallel}^2 - ((\mathbf{m}\mathbf{p}_{\parallel})^2 - (\mathbf{m}\mathbf{p}_{\perp})^2)\sin^2(0.5\nu)} \quad (5.4)$$

Obtained expression is valid when assumption that coherence amplitudes are described by homogeneous solution is true. As we would see further this assumption realized with a certain value of spin mixing angle  $\nu$ .

### 5.3.1 Evolution of Gap profile for $m_{\perp}$

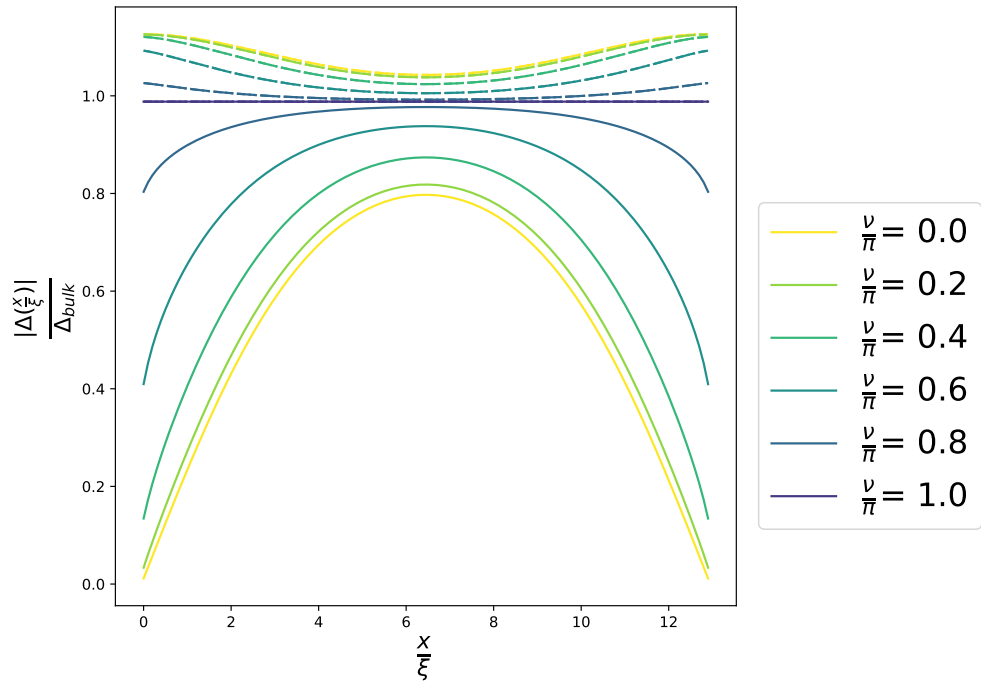
Here I consider the first case of the obtained above expression 5.4 when the magnetisation vector  $\mathbf{m} = m_{\perp}$  is perpendicular for both boundaries. This kind of magnetization of the boundaries will rotate the  $\sigma_z$  component of a Cooper pair spin projection by the angle  $\nu$ . The expression for surface states spectre will give us:

$$\frac{E}{\Delta} = \pm \sqrt{p_{\parallel}^2 + p_{\perp}^2 \sin^2(0.5\nu)}$$

The expression is showing us that in this case zero-energy states are gone and the spectrum is gapped with minimal energy  $|\sin(0.5\nu)|$ , and for  $\nu = \pi$  the bound states disappear totally,

$e = \pm\Delta$ . This indicates a complete absence of the pairbreaking. This absence is due to quasiparticle scattering in both orbital and spin spaces. This leads to effectively homogeneous order parameter along the trajectory of the quasiparticle entering the equations on coherence amplitudes.

In order to investigate this phenomenon and understand its dependence from spin a mixing angle, self-consistent calculations were performed. This allowed to obtain the order parameter dependence from a spin mixing angle. The general form of order parameter obtained for this



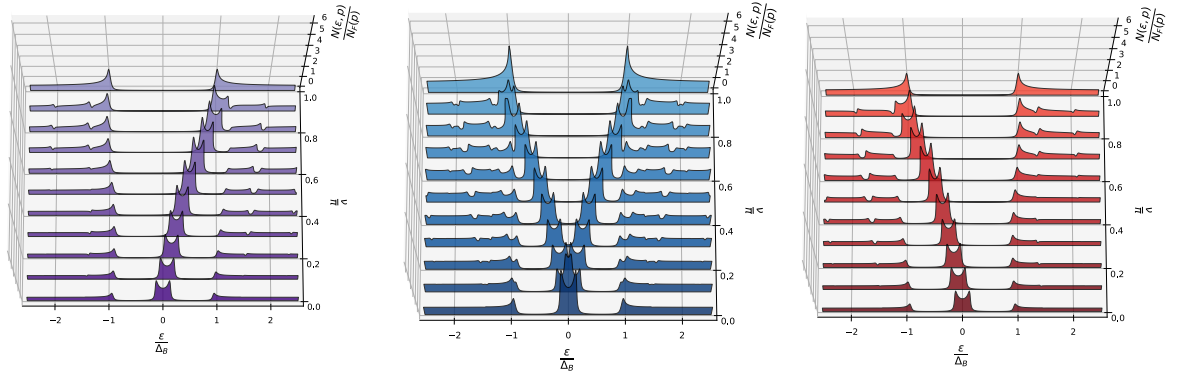
**Figure 5.5:** B phase order parameter dependence from a spin-mixing angle  $\nu$ . The dashed and dotted lines represent  $\Delta_{xx} = \Delta_{yy}$  components, while the solid line is  $\Delta_{zz}$  component.

kind of the boundary conditions:

$$\begin{pmatrix} -\Delta_1 & \Delta_2 & 0 \\ \Delta_2 & \Delta_1 & 0 \\ 0 & 0 & \Delta_3 \end{pmatrix},$$

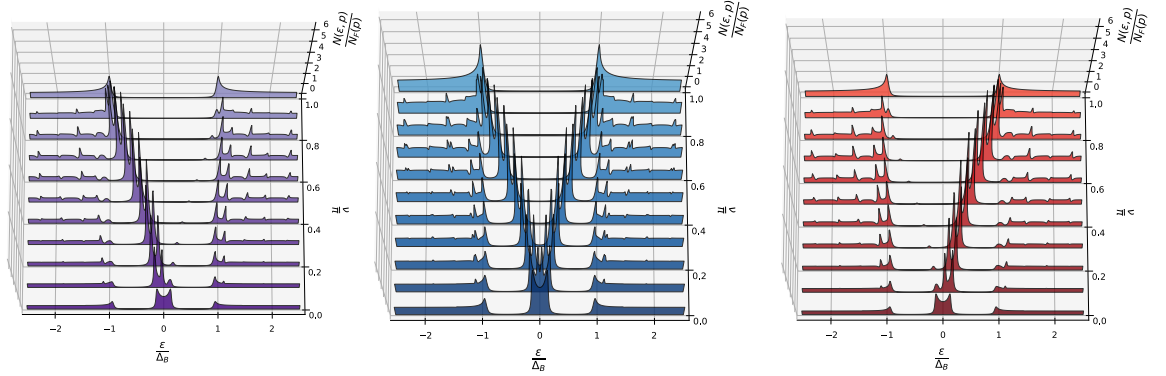
combined with the knowledge that the considered system has a rotational symmetry around  $z$  axis one could recover the form of order parameter presented at the beginning of this chapter.

In order to understand better the occurring phenomena, we can calculate the spectral local density of states for normal impact trajectory, as it is the only trajectory describing zero-energy modes has been shown in chapter 4. To cover all the possibilities for  $m_\perp$  two configurations of boundary conditions were considered. First one, that I will refer to as "parallel", is when both of the slab boundaries rotate spin components of the coherence amplitude by the same angle  $\nu$  on both boundaries. An opposite situation to the previous one would be when one of the boundaries rotates by a negative angle  $-\nu$  called "anti-parallel" consequently. As we



**Figure 5.6:** Dependence of angular resolved local density of states for spin-mixing angle  $\nu$  in the parallel case of the boundaries. Densities for spin-up, total and spin-down projections correspondingly.

can see the zero energy mode survives for small values of the parameter and any bound states vanish in the vicinity  $\nu = \pi$ , making the local density of states resemble a bulk one. One can argue as this picture valid only for given momentum direction and in case of other momenta that could be different. The answer is that only momenta involving bound states within a gap would have non-zero  $p_z$  component. For smaller  $p_z$  resonances would lie further away from zero, thus making them vanish in the continuum faster than the zero-energy state. A similar picture, but with sharper peaks observed for anti-parallel case: The difference between these two cases can be explained by leaking of Andreev bound states from the other boundary. For parallel boundary conditions, Andreev bound state from another boundary will have the same spin, thus making them repel each other, creating two close peaks that were not resolved in the first picture. For anti-parallel boundary conditions, on the other hand, leaking state would have the different spin, allowing them to pass through each other without interaction. When a helium in a slab is considered one could say that we break translational symmetry along one of the axes. By doing so, we create the conditions for the emergence of zero energy



**Figure 5.7:** Dependence of angular resolved local density of states for spin-mixing angle  $\nu$  in the anti-parallel case of the boundaries. Densities for spin-up, total and spin-down projections correspondingly.

boundary states, but if translational symmetry is somehow restored modes should vanish. That is what happens in the considered version of the problem: quasiparticle is able to be scattered preserving relative rotation of spin particles momentum, making boundary "transparent" from quasiparticles point of view. This changes the diagram, as B phase becomes stable in the whole region independently from the size of a slab as if there were no boundaries.

### 5.3.2 Evolution of Gap profile for $m_{\parallel}$

The solution obtained in this section were obtained by the gradual change of spin mixing angle on the boundaries with the B-phase as the initial condition. Attempts to obtain a solution from random initial conditions so far were unsuccessful, making me regard these solutions as local minima. Another argument against this type of solutions is that one can imagine different configuration of order parameter that minimizes the pair breaking for imposed boundary conditions:

$$\Delta \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

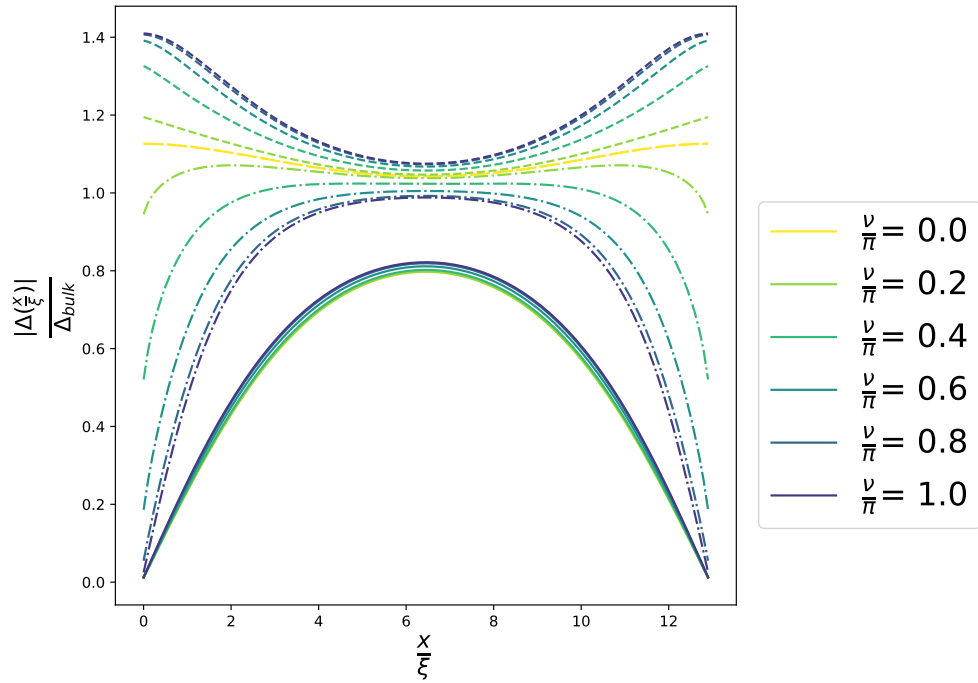
This order parameter form resembles "inverted" B-phase, and usual form can be obtained from it by rotation and flip of one of the components.

In this case, I consider magnetization of the boundary to be parallel to the boundary plane  $\mathbf{m} = m_{\parallel}$ . That kind of boundary conditions will rotate a  $\sigma_x$  component of coherence amplitudes if we choose  $x$ -axis to be directed along the  $\sigma_x$  projection of the Cooper pair spin.

The expression for surface states spectre 5.4 will give us:

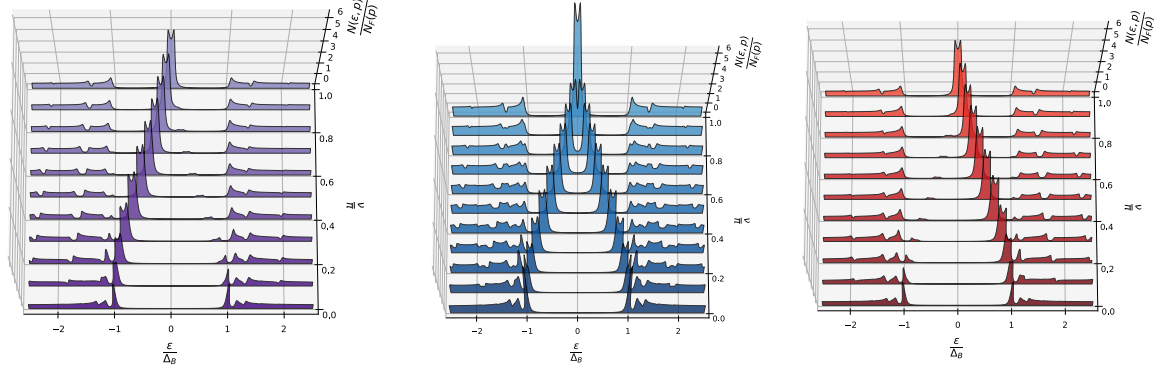
$$\frac{E}{\Delta} = \pm \sqrt{p_{\parallel}^2 - p_{\parallel}^2 \sin^2(0.5 \nu)}.$$

This expression allows to suggest that in that case we will face something similar to the B phase solution in a slab without a magnetic scattering boundaries. The calculations show us the following dependence: This time, we obtain suppression of  $\Delta_{Xx}$  component when



**Figure 5.8:** B phase order parameter dependence from a spin-mixing angle  $\nu$ . The dashed represents  $\Delta_{Yy}$  component, and the dotted line represents  $\Delta_{Xx}$  and the solid line is  $\Delta_{Zz}$  component.

$\nu = \pi$ . Plotting angular resolved local density of states, one would see that zero energy mode appeared, to be more precise it appeared for all momenta on the Fermi surface excluding those where  $p_z = 0$ , as only quasiparticles that experience reflection from the boundaries will have their x component of the spin projection flipped. This order parameter structure allows theorizing about a possibility of obtaining polar phase, if similarly to A-phase case the slab is narrow enough. This solution was obtained, but not listed here, as requiring the initial assumption at the beginning of that section to be true.



**Figure 5.9:** Dependence of angular resolved local density of states from spin-mixing angle  $\nu$ . Densities for spin-up, total and spin-down projections correspondingly.

Further, a direction of the investigation would be to consider an A-phase solution region, but this consideration is out of necessity, as it has been covered by presented data. Due to close vicinity of boundaries quasiparticles with  $p_z \neq 0$  are vanishing if  $\nu = 0$ . Leading to an inability for A-phase to react to new boundary conditions, as an average of pairs with non-zero  $p_z$  momentum goes to zero, which is  $\Delta_{\alpha z}$  by gap definition. It is easy to envision that upon the increment of  $\nu$  for a case of perpendicular magnetic orientation a boundary between A and B phase should start moving left completely disappearing for  $\nu = \pi$  with B-phase taking all space of the phase diagram. When  $m$  is parallel to the wall I also observed a polar phase, because in case of that boundary conditions in addition to  $\Delta_{\alpha z}$  component  $\Delta_{X_i}$  part is getting suppressed.

## Chapter 6

# Conclusion and outlook.

### 6.1 Summary and future prospects.

First, I would like to talk about Josephson current calculation. The considered calculation is not the first among many attempts to describe a problem of the Josephson current in systems with p-wave pairing [55]. Interest in that subject is particularly strong because of a known system of  $\text{Sr}_2\text{RuO}_4$  where it is still debatable whether the system has a p-wave pairing mechanism or some other [56]. Unlike some attempts that are just trying to describe qualitatively the effect assuming that difference in periodicity should tell the nature of coupling different approach is suggested. The approach is to exploit the effect that comes with the nature of coupling. While it is known that in s-wave condensate density of Cooper pairs is not affected by boundary effects and in d-wave systems order parameter recovers quickly for p-wave systems it can play a deciding role up to determining a state for a system to end up in. Which allows constructing such geometry that will produce the effect only in case of p-wave pairing because in both cases of d-wave and s-wave mechanisms wave function near the weak link will quickly recover and wouldn't tell the difference between the boundary conditions imposed on it on the left and right sides.

To summarize, it was a good problem to consider as it improved my knowledge of the unconventional superconductivity and developed my computational skills in terms of minimizing functions with a high number of variables. As it wasn't my main project I had to leave it in this state, but nevertheless, I consider the obtained result to be interesting and time spent on



the project fruitful as I was still considering the description of unconventional superconducting systems from the slightly different approach.

While the idea behind the problem is beautiful the implementation of it leaves with questions. First, that appears if the system considered can be approximated by its wedges or should be modelled as a whole. As we know A-phase bears a chiral current along the boundary. So could it be that the effect accounted for is actually an effect of a chiral currents going through the weak link and not cancelling each other out? To answer this question a more thorough minimization required to take a whole calculation area as shown in Fig.3.3 into account. The second question is how realistic the inner boundary condition. The reasoning behind imposing such a condition is that eventually due to destructive boundary scattering an order parameter will vanish and close to the wedge point our system will go to a normal state. Making the assumption that boundary with a normal state would be a reflective boundary close to the point of the wedge seems reasonable, but not precise as this boundary is chosen arbitrarily.

As for the second part of my thesis by the time of obtaining crucial results a publication considering the similar problem was found [57] with zero citations on it. After reading through the paper I found a few major pluses of this paper. First, I have a work which results I blindly confirmed with my calculations. As I was considering a system in a slab, author of that paper considered only a single magnetic scattering boundary. meaning, that while we agree on the same result I cover a wider variety of possibilities with my numerical approach. Second, my approach to this problem is different. My apparatus allows to calculate local densities of states which are not presented in the mentioned work. All of this makes my work a greater extension of that paper, and that might lead to an explanation why I haven't been able to obtain a global minimum solution in case of boundaries with in-plane magnetic polarization. In that case, we seem to destroy rotational symmetry around  $z$ -axis in spin space which corresponds to  $A_2$  phase, which is stable only in the presence of a magnetic field.

The second problem seems to be more perspective in terms of possible outcomes. Quite obviously one can thoroughly study all of the T-D regions in order to set dependence of a transition line between A and B phases on the spin-mixing angle. While it seems futile at this moment I can still think about the ways of obtaining a solution for crossed magnetization of the boundaries such as perpendicular on one side and parallel to surface on the other. And last but not least in order for this research to turn from a theoretical investigation of a problem

into something relevant to experimentalist one would need to establish a mechanism by which such magnetic scattering could be realized. While our preliminary estimations show that the maximum attainable value of spin-mixing angle would be  $0.1\pi$  in  $^3\text{He}$  I still think further study of possible candidates for magnetic scattering boundary is needed.

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